

Example Programs for IDA v2.4.0

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1 Introduction

This report is intended to serve as a companion document to the User Documentation of IDA [2]. It provides details, with listings, on the example programs supplied with the IDA distribution package.

The IDA distribution contains examples of four types: serial C examples, parallel C examples, and serial and parallel FORTRAN examples. The following lists summarize all of these examples.

The IDA distribution contains, in the `sundials/ida/examples_ser` directory, the following four serial examples (using the `NVECTOR_SERIAL` module):

- `idadenx` solves the Robertson chemical kinetics problem [3], which consists of two differential equations and one algebraic constraint. It also uses the rootfinding feature of IDA.

The problem is solved with the `IDADENSE` linear solver using a user-supplied Jacobian.

- `idabanx1` solves a 2-D heat equation, semidiscretized to a DAE on the unit square.

This program solves the problem with the `IDABAND` linear solver and the default difference-quotient Jacobian approximation. For purposes of illustration, `IDACalcIC` is called to compute correct values at the boundary, given incorrect values as input initial guesses. The constraint $u > 0.0$ is imposed for all components.

- `idakryx` solves the same 2-D heat equation problem as `idabanx1`, with the Krylov linear solver `IDASPGMR`. The preconditioner uses only the diagonal elements of the Jacobian.

- `idabanx2` solves a system of PDEs modelling a food web problem, with predator-prey interaction and diffusion, on the unit square in 2-D.

The PDEs are discretized in space to a system of DAEs which are solved using the `IDABAND` linear solver with the default difference-quotient Jacobian approximation.

- `idakrydem_lin` solves the same problem as `idakryx`, with three Krylov linear solvers `IDASPGMR`, `IDASPCG`, and `IDASPTFQMR`. The preconditioner uses only the diagonal elements of the Jacobian.

In the `sundials/ida/examples_par` directory, the IDA distribution contains the following four parallel examples (using the `NVECTOR_PARALLEL` module):

- `idakryx1_p` solves the same 2-D heat equation problem as `idakryx`, with `IDASPGMR` in parallel, and with a user-supplied diagonal preconditioner,

- `idakryx1_bbd_p` solves the same problem as `idakryx1_p`.

This program solves the problem in parallel, using the Krylov linear solver `IDASPGMR` and the band-block diagonal preconditioner `IDABBDPRE` with half-bandwidths equal to 1.

- `idakryx2_p` solves the same food web problem as `idabanx2`, but with `IDASPGMR` and a user-supplied preconditioner.

The preconditioner supplied to `IDASPGMR` is the block-diagonal part of the Jacobian with $n_s \times n_s$ blocks arising from the reaction terms only (n_s is the number of species in the model).

- `idakryx2_bbd_p` solves the same food web problem as `idakryx2_p`.

This program solves the problem using IDASPGMR in parallel and the IDABBDPRE preconditioner.

With the FIDA module, in the two directories `sundials/ida/fcmix/examples_ser` and `sundials/ida/fcmix/examples_par`, are the following examples for the FORTRAN-C interface:

- `fidadenx` is a serial chemical kinetics example (BDF/DENSE) with rootfinding, equivalent to `idadenx`.
- `fidakryx_bbd_p` is a parallel example (BDF/SPGMR/IDABBDPRE) equivalent to the example `idakryx1_bbd_p`.

In the following sections, we give detailed descriptions of some (but not all) of these examples. The Appendices contain complete listings of those examples described below. We also give our output files for each of these examples, but users should be cautioned that their results may differ slightly from these. Solution values may differ within tolerances, and differences in cumulative counters, such as numbers of steps or Newton iterations, may differ from one machine environment to another by as much as 10% to 20%.

In the descriptions below, we make frequent references to the IDA User Document [2]. All citations to specific sections (e.g. §5.2) are references to parts of that User Document, unless explicitly stated otherwise.

Note. The examples in the IDA distribution are written in such a way as to compile and run for any combination of configuration options during the installation of SUNDIALS (see §2). As a consequence, they contain portions of code that will not be typically present in a user program. For example, all example programs make use of the variable `SUNDIALS_EXTENDED_PRECISION` to test if the solver libraries were built in extended precision and use the appropriate conversion specifiers in `printf` functions. Similarly, the FORTRAN examples in FIDA are automatically pre-processed to generate source code that corresponds to the manner in which the IDA libraries were built (see §4 in this document for more details).

2 Serial example problems

2.1 A dense example: idadenx

This example, due to Robertson [3], is a model of a three-species chemical kinetics system written in DAE form. Differential equations are given for species y_1 and y_2 while an algebraic equation determines y_3 . The equations for the system concentrations $y_i(t)$ are:

$$\begin{cases} y'_1 &= -.04y_1 + 10^4y_2y_3 \\ y'_2 &= +.04y_1 - 10^4y_2y_3 - 3 \cdot 10^7y_2^2 \\ 0 &= y_1 + y_2 + y_3 - 1. \end{cases} \quad (1)$$

The initial values are taken as $y_1 = 1$, $y_2 = 0$, and $y_3 = 0$. This example computes the three concentration components on the interval from $t = 0$ through $t = 4 \cdot 10^{10}$. While integrating the system, the program also uses the rootfinding feature to find the points at which $y_1 = 10^{-4}$ or at which $y_3 = 0.01$.

For the source, listed in Appendix A, we give a rather detailed explanation of the parts of the program and their interaction with IDA.

Following the initial comment block, this program has a number of `#include` lines, which allow access to useful items in IDA header files. The `sundials_types.h` file provides the definition of the type `realtype` (see §5.2 in the user guide [2] for details). For now, it suffices to read `realtype` as `double`. The `ida.h` file provides prototypes for the IDA functions to be called (excluding the linear solver selection function), and also a number of constants that are to be used in setting input arguments and testing the return value of `IDASolve`. The `ida_dense.h` file provides the prototype for the `IDADense` function. The `nvector_serial.h` file is the header file for the serial implementation of the NVECTOR module and includes definitions of the `N_Vector` type, a macro to access vector components, and prototypes for the serial implementation specific machine environment memory allocation and freeing functions. Finally, note that `ida_dense.h` also includes the `sundials_dense.h` file which provides the definition of the dense matrix type `DenseMat` and a macro for accessing matrix elements.

This program includes the user-defined accessor macro `IJth` that is useful in writing the problem functions in a form closely matching the mathematical description of the DAE system, i.e. with components numbered from 1 instead of from 0. The `IJth` macro is used to access elements of a dense matrix of type `DenseMat`. It is defined using the DENSE accessor macro `DENSE_ELEM` which numbers matrix rows and columns starting with 0. The macro `DENSE_ELEM` is fully described in §5.6.4.

The program prologue ends with prototypes of the two user-supplied functions that are called by IDA and the prototype of the private function `check_flag` which is used to test the return flag from the IDA user-callable functions.

After various declarations, the `main` program begins by allocating memory for the `yy`, `yp`, and `avtol` vectors using `N_VNew_Serial` with a length argument of `NEQ` (= 3). The lines following that load the initial values of the dependent variable vectors into `yy` and `yp` and set the relative tolerance `rtol` and absolute tolerance vector `avtol`. Serial `N_Vector` values are set by first accessing the pointer to their underlying data using the macro `NV_DATA_S` defined by `NVECTOR_SERIAL` in `nvector_serial.h`.

The calls to `N_VNew_Serial`, and also later calls to IDA*** functions, make use of a private function, `check_flag`, which examines the return value and prints a message if there was a failure. This `check_flag` function was written to be used for any serial SUNDIALS application.

The call to `IDACreate` creates the IDA solver memory block. The return value of this function is a pointer to the memory block for this problem. In the case of failure, the return value is `NULL`. This pointer must be passed in the remaining calls to IDA functions.

The call to `IDAMalloc` allocates the solver memory block. Its arguments include the name of the C function `resrob` defining the residual function $F(t, y, y')$, and the initial values of t , y , and y' . The argument `IDA_SV` specifies a vector of absolute tolerances, and this is followed by the address of the relative tolerance `rtol` and the absolute tolerance vector `avtol`. See §5.5.1 for full details of this call.

The call to `IDARootInit` specifies that a rootfinding problem is to be solved along with the integration of the DAE system, that the root functions are specified in the function `grob`, and that there are two such functions. Specifically, they are set to $y_1 - 0.0001$ and $y_3 - 0.01$, respectively. See §5.7.1 for a detailed description of this call.

The calls to `IDADense` (see §5.5.3) and `IDADenseSetJacFn` (see §5.5.6.4) specify the `IDADENSE` linear solver with an analytic Jacobian supplied by the user-supplied function `jacrob`.

The actual solution of the DAE initial value problem is accomplished in the loop over values of the output time `tout`. In each pass of the loop, the program calls `IDASolve` in the `IDA_NORMAL` mode, meaning that the integrator is to take steps until it overshoots `tout` and then interpolate to $t = \text{tout}$, putting the computed value of $y(\text{tout})$ and $y'(\text{tout})$ into `yy` and `yp`, respectively, with `tret = tout`. The return value in this case is `IDA_SUCCESS`. However, if `IDASolve` finds a root before reaching the next value of `tout`, it returns `IDA_ROOT_RETURN` and stores the root location in `tret` and the solution there in `yy` and `yp`. In either case, the program prints `t` ($= tret$) and `yy`, and also the cumulative number of steps taken so far, and the current method order and step size. In the case of a root, the program calls `IDAGetRootInfo` to get a length-2 array `rootsfound` of bits showing which root function was found to have a root. If `IDASolve` returned any negative value (indicating a failure), the program breaks out of the loop. In the case of a `IDA_SUCCESS` return, the value of `tout` is advanced (multiplied by 10) and a counter (`iout`) is advanced, so that the loop can be ended when that counter reaches the preset number of output times, `NOUT = 12`. See §5.5.5 for full details of the call to `IDASolve`.

Finally, the main program calls `PrintFinalStats` to extract and print several relevant statistical quantities, such as the total number of steps, the number of residual and Jacobian evaluations, and the number of error test and convergence test failures. It then calls `IDAFree` to free the IDA memory block and `N_VDestroy_Serial` to free the vectors `yy`, `yp`, and `avtol`.

The function `PrintFinalStats` used here is actually suitable for general use in applications of IDA to any problem with a dense Jacobian. It calls various `IDAGet***` and `IDADenseGet***` functions to obtain the relevant counters, and then prints them. Specifically, these are: the cumulative number of steps (`nst`), the number of residual evaluations (`nre`) (excluding those for difference-quotient Jacobian evaluations), the number of residual evaluations for Jacobian evaluations (`nreLS`), the number of Jacobian evaluations (`nje`), the number of nonlinear (Newton) iterations (`nni`), the number of local error test failures (`netf`), the number of nonlinear convergence failures (`ncfn`), and the number of `grob` (root function) evaluations (`nge`). These optional outputs are described in §5.5.8.

The functions `resrob` (of type `IDAResFn`) and `jacrob` (of type `IDADenseJacFn`) are straightforward expressions of the DAE system (1) and its system Jacobian. The function `jacrob` makes use of the macro `IJth` discussed above. See §5.6.1 for detailed specifications of `IDAResFn`. Similarly, the function `grob` defines the two functions, g_0 and g_1 , whose roots are to be found. See §5.7.2 for a detailed description of the `grob` function.

The output generated by `idadenx` is shown below. It shows the output values at the 12 preset values of `tout`. It also shows the two root locations found, first at a root of g_1 , and then at a root of g_0 .

```
----- idadenx sample output -----
idadenx: Robertson kinetics DAE serial example problem for IDA
Three equation chemical kinetics problem.

Linear solver: IDADENSE, with user-supplied Jacobian.
Tolerance parameters: rtol = 0.0001 atol = 1e-08 1e-14 1e-06
Initial conditions y0 = (1 0 0)
Constraints and id not used.

-----
t          y1          y2          y3    | nst   k     h
-----
2.6403e-01  9.8997e-01  3.4706e-05  1.0000e-02 | 85   2   6.4537e-02
rootsfound[] = 0   1
4.0000e-01  9.8517e-01  3.3864e-05  1.4796e-02 | 88   2   6.4537e-02
4.0000e+00  9.0550e-01  2.2403e-05  9.4473e-02 | 102  4   4.1426e-01
4.0000e+01  7.1582e-01  9.1851e-06  2.8417e-01 | 136  2   1.3422e+00
4.0000e+02  4.5049e-01  3.2226e-06  5.4950e-01 | 190  4   3.3557e+01
4.0000e+03  1.8321e-01  8.9429e-07  8.1679e-01 | 239  4   3.4533e+02
4.0000e+04  3.8984e-02  1.6218e-07  9.6102e-01 | 287  5   2.0140e+03
4.0000e+05  4.9389e-03  1.9852e-08  9.9506e-01 | 339  3   1.6788e+04
4.0000e+06  5.1683e-04  2.0684e-09  9.9948e-01 | 444  4   2.1755e+05
2.0793e+07  1.0000e-04  4.0004e-10  9.9990e-01 | 495  4   1.0146e+06
rootsfound[] = 1   0
4.0000e+07  5.2036e-05  2.0816e-10  9.9995e-01 | 506  5   2.5503e+06
4.0000e+08  5.2103e-06  2.0841e-11  9.9999e-01 | 541  4   2.3847e+07
4.0000e+09  5.2125e-07  2.0850e-12  1.0000e-00 | 569  4   3.9351e+08
4.0000e+10  5.1091e-08  2.0437e-13  1.0000e-00 | 589  2   6.0246e+09

Final Run Statistics:

Number of steps                      = 589
Number of residual evaluations        = 832
Number of Jacobian evaluations       = 79
Number of nonlinear iterations       = 832
Number of error test failures       = 14
Number of nonlinear conv. failures  = 0
Number of root fn. evaluations      = 631
```

2.2 A banded example: `idabanx2`

This example is a model of a multi-species food web [1], in which predator-prey relationships with diffusion in a 2-D spatial domain are simulated. Here we consider a model with $s = 2p$ species: p predators and p prey. Species $1, \dots, p$ (the prey) satisfy rate equations, while species $p + 1, \dots, s$ (the predators) have infinitely fast reaction rates. The coupled PDEs for the species concentrations $c^i(x, y, t)$ are:

$$\begin{cases} \partial c^i / \partial t = R_i(x, y, c) + d_i(c_{xx}^i + c_{yy}^i) & i = 1, 2, \dots, p \\ 0 = R_i(x, y, c) + d_i(c_{xx}^i + c_{yy}^i) & i = p + 1, \dots, s \end{cases}, \quad (2)$$

with

$$R_i(x, y, c) = c^i \left(b_i + \sum_{j=1}^s a_{ij} c^j \right).$$

Here c denotes the vector $\{c^i\}$. The interaction and diffusion coefficients (a_{ij}, b_i, d_i) can be functions of (x, y) in general. The choices made for this test problem are as follows:

$$a_{ij} = \begin{cases} -1 & i = j \\ -0.5 \cdot 10^{-6} & i \leq p, j > p \\ 10^4 & i > p, j \leq p \\ 0 & \text{all other } (i, j), \end{cases}$$

$$b_i = b_i(x, y) = \begin{cases} (1 + \alpha xy + \beta \sin(4\pi x) \sin(4\pi y)) & i \leq p \\ -(1 + \alpha xy + \beta \sin(4\pi x) \sin(4\pi y)) & i > p, \end{cases}$$

and

$$d_i = \begin{cases} 1 & i \leq p \\ 0.5 & i > p. \end{cases}$$

The spatial domain is the unit square $0 \leq x, y \leq 1$, and the time interval is $0 \leq t \leq 1$. The boundary conditions are of homogeneous Neumann type (zero normal derivatives) everywhere. The coefficients are such that a unique stable equilibrium is guaranteed to exist when $\alpha = \beta = 0$ [1]. Empirically, a stable equilibrium appears to exist for (2) when α and β are positive, although it may not be unique. In this problem we take $\alpha = 50$ and $\beta = 1000$. For the initial conditions, we set each prey concentration to a simple polynomial profile satisfying the boundary conditions, while the predator concentrations are all set to a flat value:

$$c^i(x, y, 0) = \begin{cases} 10 + i[16x(1-x)y(1-y)]^2 & i \leq p, \\ 10^5 & i > p. \end{cases}$$

We discretize this PDE system (2) (plus boundary conditions) with central differencing on an $L \times L$ mesh, so as to obtain a DAE system of size $N = sL^2$. The dependent variable vector C consists of the values $c^i(x_j, y_k, t)$ grouped first by species index i , then by x , and lastly by y . At each spatial mesh point, the system has a block of p ODE's followed by a block of p algebraic equations, all coupled. For this example, we take $p = 1, s = 2$, and $L = 20$. The Jacobian is banded, with half-bandwidths $\text{mu} = \text{ml} = sL = 40$.

The `idabanx2.c` program (listed in Appendix B) includes the file `ida_band.h` in order to use the IDABAND linear solver. This file contains the prototype for the `IDABand` routine, the definition for the band matrix type `BandMat`, and the `BAND_COL` and `BAND_COL_ELEM` macros for accessing matrix elements. See §9.2. The main IDA header file `ida.h` is included for the prototypes of the solver user-callable functions and IDA constants, while the file `nvector_serial.h` is included for the definition of the serial `N_Vector` type. The header file `sundials_smalldense.h` is included for the `denalloc` function used in allocating memory for the user data structure.

The include lines at the top of the file are followed by definitions of problem constants which include the x and y mesh dimensions, `MX` and `MY`, the number of equations `NEQ`, the scalar relative and absolute tolerances `RTOL` and `ATOL`, and various parameters for the food-web problem.

Spatial discretization of the PDE naturally produces a DAE system in which equations are numbered by mesh coordinates (i, j) . The user-defined macro `IJth_Vptr` isolates the translation for the mathematical two-dimensional index to the one-dimensional `N_Vector` index and allows the user to write clean, readable code to access components of the dependent variable. `IJ_Vptr(v, i, j)` returns a pointer to the location in `v` corresponding to the species with index `is = 0`, x-index `ix = i`, and y-index `jy = j`.

The type `UserData` is a pointer to a structure containing problem data used in the `resweb` function. This structure is allocated and initialized at the beginning of `main`. The pointer to it, called `webdata`, is then passed to `IDASetRData` and as a result it will be passed back to the `resweb` function each time it is called.

The `main` program is straightforward and very similar to that for `idadenx`. The differences come from the use of the IDABAND linear solver and from the use of the consistent initial conditions algorithm in IDA to correct the initial values. `IDACalcIC` is called with the option `IDA_YA_YDP_INIT`, meaning that IDA is to compute the algebraic components of y and differential components of y' , given the differential components of y . This option requires that the `N_Vector` `id` be set through a call to `IDASetId` specifying the differential and algebraic components. In this example, `id` has components equal to 1 for the prey (indicating differential variables) and 0 for the predators (algebraic variables).

Next, the `IDASolve` function is called in a loop over the output times, and the solution for the species concentrations at the bottom-left and top-right corners is printed, along with the cumulative number of time steps, current method order, and current step size.

Finally, the main program calls `PrintFinalStats` to get and print all of the relevant statistical quantities. It then calls `N_VDestroy_Serial` to free the vectors `cc`, `cp`, and `id`, and `IDAFree` to free the IDA memory block.

The function `PrintFinalStats` used here is actually suitable for general use in applications of IDA to any problem with a banded Jacobian. It calls various `IDAGet***` and `IDABandGet***` functions to obtain the relevant counters, and then prints them. Specifically, these are: the cumulative number of steps (`nst`), the number of residual evaluations (`nre`) (excluding those for difference-quotient Jacobian evaluations), the number of residual evaluations for Jacobian evaluations (`nreLS`), the number of Jacobian evaluations (`nje`), the number of nonlinear (Newton) iterations (`nni`), the number of local error test failures (`netf`), and the number of nonlinear convergence failures (`ncfn`). These optional outputs are described in §5.5.8.

The function `resweb` is a direct translation of the residual of (2). It first calls the private function `Fweb` to initialize the residual vector with the right-hand side of (2) and then it loops over all grid points, setting residual values appropriately for differential or algebraic components. The calculation of the interaction terms R_i is done in the function `WebRates`.

Sample output from `idabanx2` follows.

idabanx2 sample output

```

idabanx2: Predator-prey DAE serial example problem for IDA

Number of species ns: 2      Mesh dimensions: 20 x 20      System size: 800
Tolerance parameters: rtol = 1e-05    atol = 1e-05
Linear solver: IDABAND, Band parameters mu = 40, ml = 40
CalcIC called to correct initial predator concentrations.

-----
t      bottom-left   top-right   | nst   k       h
-----
```

```

-----
0.00e+00  1.0000e+01  9.9949e+04 | 0 0 1.6310e-08
                                9.9999e+04 9.9949e+04 |

1.00e-03  1.0318e+01  1.0822e+05 | 32 4 1.0823e-04
                                1.0319e+05 1.0822e+05 |

1.00e-02  1.6189e+02  1.9735e+06 | 135 4 1.7964e-04
                                1.6189e+06 1.9735e+06 |

1.00e-01  2.4019e+02  2.7072e+06 | 231 1 4.4212e-02
                                2.4019e+06 2.7072e+06 |

4.00e-01  2.4019e+02  2.7072e+06 | 233 1 1.7685e-01
                                2.4019e+06 2.7072e+06 |

7.00e-01  2.4019e+02  2.7072e+06 | 234 1 3.5370e-01
                                2.4019e+06 2.7072e+06 |

1.00e+00  2.4019e+02  2.7072e+06 | 235 1 7.0740e-01
                                2.4019e+06 2.7072e+06 |

-----
Final run statistics:

Number of steps = 235
Number of residual evaluations = 3319
Number of Jacobian evaluations = 36
Number of nonlinear iterations = 401
Number of error test failures = 5
Number of nonlinear conv. failures = 0

```

2.3 A Krylov example: `idakryx`

This example solves a discretized 2D heat PDE problem. The DAE system arises from the Dirichlet boundary condition $u = 0$, along with the differential equations arising from the discretization of the interior of the region.

The domain is the unit square $\Omega = \{0 \leq x, y \leq 1\}$ and the equations solved are:

$$\begin{cases} \partial u / \partial t = u_{xx} + u_{yy} & (x, y) \in \Omega \\ u = 0 & (x, y) \in \partial\Omega . \end{cases} \quad (3)$$

The time interval is $0 \leq t \leq 10.24$, and the initial conditions are $u = 16x(1-x)y(1-y)$.

We discretize the PDE system (3) (plus boundary conditions) with central differencing on a 10×10 mesh, so as to obtain a DAE system of size $N = 100$. The dependent variable vector u consists of the values $u(x_j, y_k, t)$ grouped first by x , and then by y . Each discrete boundary condition becomes an algebraic equation within the DAE system.

The source for this example is listed in Appendix C. In this case, `ida_spgmr.h` is included for the definitions of constants and function prototypes associated with the SPGMR method.

After various initializations (including a vector of constraints with all components set to 1 imposing all solution components to be non-negative), the main program creates and initializes the IDA memory block and then attaches the IDASPGMR linear solver using the default `MODIFIED_GS` Gram-Schmidt orthogonalization algorithm.

The calls to `IDASpgmrSetPrecSetupFn` and `IDASpgmrSetPsolveFn` specify the use of the user-supplied preconditioner with `data` being the pointer to user data passed to `PsolveHeat` and `PsetupHeat` whenever they are called (specified with the call to `IDASpgmrSetPrecData`). In a loop over the desired output times, `IDASolve` is called in `IDA_NORMAL` mode and the maximum solution norm is printed.

The `main` program then re-initializes the IDA solver and the IDASPGMR linear solver and solves the problem again, this time using the `CLASSICAL_GS` Gramm-Schmidt orthogonalization algorithm. Finally, memory for the IDA solver and for the various vectors used is deallocated.

The user-supplied residual function `resHeat`, of type `IDAResFn`, loads the DAE residual with the value of u on the boundary (representing the algebraic equations expressing the boundary conditions of (3)) and with the spatial discretization of the PDE (using central differences) in the rest of the domain.

The user-supplied functions `PsetupHeat` and `PsolveHeat` together define the left preconditioner matrix P approximating the system Jacobian matrix $J = \partial F / \partial u + \alpha \partial F / \partial u'$ (where the DAE system is $F(t, u, u') = 0$), and solve the linear systems $Pz = r$. Preconditioning is done in this case by keeping only the diagonal elements of the J matrix above, storing them as inverses in a vector `pp`, when computed in `PsetupHeat`, for subsequent use in `PsolveHeat`. In this instance, only `cj = alpha` and `data` (the user data structure) are used from the `PsetupHeat` argument list.

Sample output from `idakryx` follows.

```
----- idakryx sample output -----  
  
idakryx: Heat equation, serial example problem for IDA  
Discretized heat equation on 2D unit square.  
Zero boundary conditions, polynomial initial conditions.  
Mesh dimensions: 10 x 10      Total system size: 100  
  
Tolerance parameters: rtol = 0    atol = 0.001  
Constraints set to force all solution components >= 0.  
Linear solver: IDASPGMR, preconditioner using diagonal elements.  
  
Case 1: gsytype = MODIFIED_GS  
  
Output Summary (umax = max-norm of solution)  
  
time      umax       k     nst     nni     nje     nre     nreLS      h      npe     nps  
-----  
0.01      8.24106e-01   2     12     14      7     14      7    2.56e-03     8     21  
0.02      6.88134e-01   3     15     18     12     18     12    5.12e-03     8     30  
0.04      4.70711e-01   3     18     24     21     24     21    6.58e-03     9     45  
0.08      2.16509e-01   3     22     29     30     29     30    1.32e-02     9     59  
0.16      4.57687e-02   4     28     36     44     36     44    1.32e-02     9     80  
0.32      2.09938e-03   4     35     44     67     44     67    2.63e-02    10    111  
0.64      0.00000e+00   1     39     51     77     51     77    1.05e-01    12    128  
1.28      0.00000e+00   1     41     53     77     53     77    4.21e-01    14    130  
2.56      0.00000e+00   1     43     55     77     55     77    1.69e+00    16    132  
5.12      0.00000e+00   1     44     56     77     56     77    3.37e+00    17    133  
10.24     0.00000e+00   1     45     57     77     57     77    6.74e+00   18    134  
  
Error test failures          = 1  
Nonlinear convergence failures = 0
```

Linear convergence failures	= 0								
Case 2: gstype = CLASSICAL_GS									
Output Summary (umax = max-norm of solution)									
time	umax	k	nst	nni	nje	nre	nreLS	h	npe nps
0.01	8.24106e-01	2	12	14	7	14	7	2.56e-03	8 21
0.02	6.88134e-01	3	15	18	12	18	12	5.12e-03	8 30
0.04	4.70711e-01	3	18	24	21	24	21	6.58e-03	9 45
0.08	2.16509e-01	3	22	29	30	29	30	1.32e-02	9 59
0.16	4.57687e-02	4	28	36	44	36	44	1.32e-02	9 80
0.32	2.09938e-03	4	35	44	67	44	67	2.63e-02	10 111
0.64	5.54028e-21	1	39	51	77	51	77	1.05e-01	12 128
1.28	5.77661e-20	1	41	53	77	53	77	4.21e-01	14 130
2.56	1.00105e-19	1	43	55	77	55	77	1.69e+00	16 132
5.12	3.17879e-19	1	44	56	77	56	77	3.37e+00	17 133
10.24	9.19490e-19	1	45	57	77	57	77	6.74e+00	18 134
Error test failures	= 1								
Nonlinear convergence failures	= 0								
Linear convergence failures	= 0								

3 Parallel example problems

3.1 A user preconditioner example: `idakryx1_p`

As an example of using IDA with the parallel MPI NVECTOR_PARALLEL module and the Krylov linear solver IDASPGMR with user-defined preconditioner, we provide the example `idakryx1_p` which solves the same 2-D heat PDE problem as `idakryx`. The source is listed in Appendix D.

In the parallel setting, we can think of the processors as being laid out in a grid of size `NPEX × NPEY`, with each processor computing a subset of the solution vector on a submesh of size `MXSUB × MYSUB`. As a consequence, the computation of the residual vector requires that each processor exchange boundary information (namely the components at all interior subgrid boundaries) with its neighboring processors. The message-passing (implemented in the function `rescomm`) uses blocking sends, non-blocking receives, and receive-waiting, in routines `BSend`, `BRecvPost`, and `BRecvWait`, respectively. The data received from each neighboring processor is then loaded into a work array, `uext`, which contains this ghost cell data along with the local portion of the solution.

The local portion of the residual vector is then computed in the routine `reslocal`, which assumes that all inter-processor communication of data needed to calculate `rr` has already been done. Components at interior subgrid boundaries are assumed to be in the work array `uext`. The local portion of the solution vector `uu` is first copied into `uext`. The diffusion terms are evaluated in terms of the `uext` array, and the residuals are formed. The zero Dirichlet boundary conditions are handled here by including the boundary components in the residual, giving algebraic equations for the discrete boundary conditions.

The preconditioner (`PsolveHeat` and `PsetupHeat`) uses the diagonal elements of the Jacobian only and therefore involves only local calculations.

The `idakryx1_p` main program begins with MPI calls to initialize MPI and to set multi-processor environment parameters `npes` (number of processes) and `thispe` (local process index). Then the local and global vector lengths are set, the user-data structure `Userdata` is created and initialized, and `N_Vector` variables are created and initialized for the initial conditions (`uu` and `up`), for the vector `id` specifying the differential and algebraic components of the solution vector, and for the preconditioner (`pp`). As in `idakryx`, constraints are passed to IDA through the `N_Vector constraints` and the function `IDASetConstraints`. A temporary `N_Vector res` is also created here, for use only in `SetInitialProfiles`. All components of `constraints` are set to 1.0 indicating that non-negativity constraints are to be imposed on each solution component. In addition, for illustration purposes, `idakryx` also excludes the algebraic components of the solution (specified through the `N_Vector id`) from the error test by calling `IDASetSuppressAlg` with a flag TRUE.

Sample output from `idakryx1_p` follows.

```
----- idakryx1_p sample output -----  
  
idakryx1_p: Heat equation, parallel example problem for IDA  
Discretized heat equation on 2D unit square.  
Zero boundary conditions, polynomial initial conditions.  
Mesh dimensions: 10 x 10      Total system size: 100  
  
Subgrid dimensions: 5 x 5      Processor array: 2 x 2  
Tolerance parameters: rtol = 0    atol = 0.001  
Constraints set to force all solution components >= 0.
```

```

SUPPRESSALG = TRUE to suppress local error testing on all boundary components.
Linear solver: IDASPGMR  Preconditioner: diagonal elements only.

Output Summary (umax = max-norm of solution)

  time      umax      k     nst     nni     nli     nre     nreLS      h      npe     nps
-----
  0.00  9.75461e-01  0     0     0     0     0     0   0.00e+00  0     0
  0.01  8.24106e-01  2    12    14     7    14     7   2.56e-03  8    21
  0.02  6.88134e-01  3    15    18    12    18     12   5.12e-03  8    30
  0.04  4.70711e-01  3    18    24    21    24     21   6.58e-03  9    45
  0.08  2.16509e-01  3    22    29    30    29     30   1.32e-02  9    59
  0.16  4.57687e-02  4    28    36    44    36     44   1.32e-02  9    80
  0.32  2.09938e-03  4    35    44    67    44     67   2.63e-02 10   111
  0.64  0.00000e+00  1    39    51    77    51     77   1.05e-01 12   128
  1.28  0.00000e+00  1    41    53    77    53     77   4.21e-01 14   130
  2.56  0.00000e+00  1    43    55    77    55     77   1.69e+00 16   132
  5.12  0.00000e+00  1    44    56    77    56     77   3.37e+00 17   133
 10.24  0.00000e+00  1    45    57    77    57     77   6.74e+00 18   134

Error test failures          = 1
Nonlinear convergence failures = 0
Linear convergence failures  = 0

```

3.2 An IDABBDPRE preconditioner example: `idakryx2_bbd_p`

In this example, `idakryx2_bbd_p`, we solve the same food web problem as with `idabanx2`, but in parallel and with the IDASPGMR linear solver and using the IDABBDPRE module, which generates and uses a band-block-diagonal preconditioner. The source is listed in Appendix E.

As with `idakryx1_p`, we use a NPEX \times NPEY processor grid, with an MXSUB \times MYSUB submesh on each processor. Again, the residual evaluation begins with the communication of ghost data (in `rescomm`), followed by computation using an extended local array, `cext`, in the `reslocal` routine. The exterior Neumann boundary conditions are explicitly handled here by copying data from the first interior mesh line to the ghost cell locations in `cext`. Then the reaction and diffusion terms are evaluated in terms of the `cext` array, and the residuals are formed.

The Jacobian block on each processor is banded, and the half-bandwidths of that block are both equal to `NUM_SPECIES` · MXSUB. This is the value supplied as `mudq` and `mldq` in the call to `IDABBDPrecAlloc`. But in order to reduce storage and computation costs for preconditioning, we supply the values `mukeep` = `mlkeep` = 2 (= `NUM_SPECIES`) as the half-bandwidths of the retained band matrix blocks. This means that the Jacobian elements are computed with a difference quotient scheme using the true bandwidth of the block, but only a narrow band matrix (bandwidth 5) is kept as the preconditioner.

The function `reslocal` is also passed to the IDABBDPRE preconditioner as the `Gres` argument, while a NULL pointer is passed for the `Gcomm` argument (since all required communication for the evaluation of `Gres` was already done for `resweb`).

In the `idakryx2_bbd_p` main program, following MPI initializations and creation of user data block `webdata` and `N_Vector` variables, the initial profiles are set, the IDA memory block is created and allocated, the IDABBDPRE preconditioner is initialized, and the IDASPGMR linear solver is attached to the IDA solver. The call to `IDACalcIC` corrects the initial values so that they are consistent with the DAE algebraic constraints.

In a loop over the desired output times, the main solver function `IDASolve` is called, and selected solution components (at the bottom-left and top-right corners of the computational domain) are collected on processor 0 and printed to `stdout`. The main program ends by printing final solver statistics, freeing memory, and finalizing MPI.

Sample output from `idakryx2_bbd_p` follows.

```
----- idakryx2_bbd_p sample output -----
idakryx2_bbd_p: Predator-prey DAE parallel example problem

Number of species ns: 2
Mesh dimensions:      20 x 20
Total system size:    800
Subgrid dimensions:   10 x 10
Processor array:       2 x 2
Tolerance parameters:
  relative tolerance = 1e-05
  absolute tolerance = 1e-05
Linear solver: scaled preconditioned GMRES (IDASPGMR)
  max. Krylov dimension: maxl = 12
Preconditioner: band-block-diagonal (IDABBDPRE)
  mldq = 20,  mldq = 20,  mukeep = 2,  mlkeep = 2
CalcIC called to correct initial predator concentrations

-----
t      bottom-left   top-right   | nst   k     h
-----
0.00e+00  1.0000e+01  1.0000e+01  |  0   0   1.6310e-08
                           9.9999e+04  9.9949e+04  |
1.00e-03  1.0318e+01  1.0827e+01  |  33   4   9.7404e-05
                           1.0319e+05  1.0822e+05  |
1.00e-02  1.6189e+02  1.9735e+02  | 125   3   9.7404e-05
                           1.6189e+06  1.9735e+06  |
1.00e-01  2.4019e+02  2.7072e+02  | 201   1   4.0396e-02
                           2.4019e+06  2.7072e+06  |
4.00e-01  2.4019e+02  2.7072e+02  | 204   1   3.2316e-01
                           2.4019e+06  2.7072e+06  |
7.00e-01  2.4019e+02  2.7072e+02  | 205   1   6.4633e-01
                           2.4019e+06  2.7072e+06  |
1.00e+00  2.4019e+02  2.7072e+02  | 205   1   6.4633e-01
                           2.4019e+06  2.7072e+06  |

-----
Final statistics:

Number of steps                  = 205
Number of residual evaluations   = 1279
Number of nonlinear iterations   = 253
Number of error test failures   = 0
Number of nonlinear conv. failures = 0
```

Number of linear iterations	= 1024
Number of linear conv. failures	= 0

Number of preconditioner setups	= 25
Number of preconditioner solves	= 1279
Number of local residual evals.	= 1050

4 Fortran example problems

The FORTRAN example problem programs supplied with the IDA package are all written in standard FORTRAN77 and use double precision arithmetic. However, when the FORTRAN examples are built, the source code is automatically modified according to the configure options supplied by the user and the system type. Integer variables are declared as `INTEGER*n`, where n denotes the number of bytes in the corresponding C type (`long int` or `int`). Floating-point variable declarations remain unchanged if double precision is used, but are changed to `REAL*n`, where n denotes the number of bytes in the SUNDIALS type `realtype`, if using single-precision. Also, if using single-precision, then declarations of floating-point constants are appropriately modified; e.g. `0.5D-4` is changed to `0.5E-4`.

4.1 A serial example: fidadenx

The `fidadenx` example is a FORTRAN equivalent of the `idadenx` problem. The source program `fidadenx.f` is listed in Appendix F.

The main program begins with declarations and initializations. It calls the routines `FNVINITS`, `FIDAMALLOC`, `FIDAROOTINIT`, `FIDADENSE`, and `FIDADENSESETJAC`, to initialize the `NVECTOR_SERIAL` module, the main solver memory, the rootfinding module, and the `IDADENSE` module, and to specify user-supplied Jacobian routine, respectively. It calls `FIDASOLVE` in a loop over `TOUT` values, with printing of the solution values and performance data (current order and step count from the `IOUT` array, and current step size from the `ROUT` array). In the case of a root return, an extra line is printed with the root information from `FIDAROOTINFO`. At the end, it prints a number of performance counters, and frees memory with calls to `FIDAROOTFREE` and `FIDAFREE`.

In `fidadenx.f`, the `FIDARESFUN` routine is a straightforward implementation of Eqns. (1). In `FIDADJAC`, the 3×3 system Jacobian is supplied. The `FIDAROOTFN` routine defines the two root functions, which are set to determine the points at which $y_1 = 10^{-4}$ or $y_3 = .01$. The final two routines are for the printing of a header and of the final run statistics.

The following is sample output from `fidadenx`. The performance of FIDA here is similar to that of IDA on the `idadenx` problem, with somewhat lower cost counters owing to the larger absolute error tolerances.

```
fidadenx sample output

fidadenx: Robertson kinetics DAE serial exampleproblem for IDA
          Three equation chemcalkinetics problem.

Tolerance parameters: rtol = 0.10E-03    atol =  0.10E-05 0.10E-09 0.10E-05
Initial conditions y0 = ( 0.10E+01 0.00E+00 0.00E+00)

      t            y1            y2            y3            nst      k      h
0.2640E+00  0.9900E+00  0.3471E-04  0.1000E-01    75      2  0.5716E-01
      Above is a root, INFO() = 0 1
0.4000E+00  0.9852E+00  0.3386E-04  0.1480E-01    77      3  0.1143E+00
0.4000E+01  0.9055E+00  0.2240E-04  0.9447E-01    91      4  0.3704E+00
0.4000E+02  0.7158E+00  0.9185E-05  0.2842E+00   127      4  0.2963E+01
0.4000E+03  0.4505E+00  0.3223E-05  0.5495E+00   177      3  0.1241E+02
0.4000E+04  0.1832E+00  0.8940E-06  0.8168E+00   228      3  0.2765E+03
0.4000E+05  0.3899E-01  0.1622E-06  0.9610E+00   278      5  0.2614E+04
0.4000E+06  0.4939E-02  0.1985E-07  0.9951E+00   324      5  0.2770E+05
0.4000E+07  0.5176E-03  0.2072E-08  0.9995E+00   355      4  0.3979E+06
```

```

0.2075E+08   0.1000E-03   0.4000E-09   0.9999E+00   374   4   0.1592E+07
      Above is a root, INFO() = 1 0
0.4000E+08   0.5191E-04   0.2076E-09   0.9999E+00   380   3   0.6366E+07
0.4000E+09   0.5882E-05   0.2353E-10   0.1000E+01   394   1   0.9167E+08
0.4000E+10   0.7054E-06   0.2822E-11   0.1000E+01   402   1   0.1467E+10
0.4000E+11   -0.7300E-06   -0.2920E-11   0.1000E+01   407   1   0.2347E+11

Final Run Statistics:

Number of steps                      = 407
Number of residual evaluations        = 557
Number of Jacobian evaluations       = 65
Number of nonlinear iterations       = 557
Number of error test failures       = 6
Number of nonlinear conv. failures  = 0
Number of root function evals.     = 437

```

4.2 A parallel example: fidakryx_bbd_p

This example, `fidakryx_bbd_p`, is the FORTRAN equivalent of the `idakryx1_bbd_p` example. The heat equation problem is described under the `idakryx` example above, but here it is solved in parallel, using the IDABBDPRE (band-block-diagonal) preconditioner module. The decomposition of the problem onto a processor array is identical to that in the `idakryx1_p` example above. The source file, `fidakryx_bbd_p.f`, is listed in Appendix G.

The problem is solved twice — once with half-bandwidths of 5 in the difference-quotient banded preconditioner blocks, and once with half-bandwidths of 1 (which results in lumping of Jacobian values). In both cases, the retained banded blocks are tridiagonal, even though the true Jacobian is not.

The main program begins with initializations, including MPI calls, a call to FNVINITP to initialize NVECTOR_PARALLEL, and a call to SETINITPROFILE to initialize the UU, UP, ID, and CONSTR arrays (containing the solution vector, solution derivative vector, the differential/algebraic bit vector, and the constraint specification vector, respectively). A call to FIDASETIIN and two calls to FIDASETVIN are made to suppress error control on the algebraic variables, and to supply the ID array and constraints array (making the computed solution non-negative). The call to FIDAMALLOC initializes the FIDA main memory, and the calls to FIDABBDINIT and FIDABBDSPGMR initialize the FIDABBD module.

In the first loop over TOUT values, the main program calls FIDASOLVE and prints the max-norm of the solution and selected counters. When finished, it calls PRNTFINALSTATS to print a few more counters.

The second solution is initialized by a second call to SETINITPROFILE, and calls to FIDAREINIT and FIDABBDREINIT. After completing the second solution, the program frees memory and terminates MPI.

The `FIDARESFUN` routine simply calls two other routines: `FIDACOMMFN`, to communicate boundary needed data from U to an extension of it called UEXT; and `FIDAGLOCFN`, to compute the residuals in terms of UEXT and UP.

The following is a sample output from `fidakryx_bbd_p`, with a 10×10 mesh and $NPES = 4$ processors. The performance is similar for the two solutions. The second case requires more linear iterations, as expected, but their cost is offset by the much cheaper preconditioner evaluations.

fidakryx_bbd_p sample output

```
fidakryx_bbd_p: Heat equation, parallel example problem for FIDA
Discretized heat equation on 2D unit square.
Zero boundary conditions, polynomial conditions.
Mesh dimensions: 10 x 10           Total system size: 100

Subgrid dimensions: 5 x 5          Processor array: 2 x 2
Tolerance parameters: rtol = 0.00E+00  atol = 0.10E-02
Constraints set to force all solution components >= 0.
SUPPRESSALG = TRUE to remove boundary components from the error test.
Linear solver: SPGMR.    Preconditioner: BBDPRE - Banded-block-diagonal.
```

Case 1

```
Difference quotient half-bandwidths = 5
Retained matrix half-bandwidths = 1
```

Output Summary

```
umax = max-norm of solution
nre = nre + nreLS (total number of RES evals.)
```

time	umax	k	nst	nni	nli	nre	nge	h	npe	nps
0.1000E-01	0.82411E+00	2	12	14	7	14+ 7	96	0.26E-02	8	21
0.2000E-01	0.68812E+00	3	15	18	12	18+12	96	0.51E-02	8	30
0.4000E-01	0.47075E+00	3	18	24	22	24+22	108	0.66E-02	9	46
0.8000E-01	0.21660E+00	3	22	29	30	29+30	108	0.13E-01	9	59
0.1600E+00	0.45659E-01	4	28	37	43	37+43	120	0.26E-01	10	80
0.3200E+00	0.21096E-02	4	35	45	59	45+59	120	0.24E-01	10	104
0.6400E+00	0.50233E-04	1	40	54	70	54+70	156	0.19E+00	13	124
0.1280E+01	0.23658E-18	1	42	56	70	56+70	180	0.76E+00	15	126
0.2560E+01	0.14313E-19	1	43	57	70	57+70	192	0.15E+01	16	127
0.5120E+01	0.42389E-19	1	44	58	70	58+70	204	0.30E+01	17	128
0.1024E+02	0.99241E-19	1	45	59	70	59+70	216	0.61E+01	18	129

```
Error test failures      = 1
Nonlinear convergence failures = 0
Linear convergence failures = 0
```

Case 2

```
Difference quotient half-bandwidths = 1
Retained matrix half-bandwidths = 1
```

Output Summary

```
umax = max-norm of solution
nre = nre + nreLS (total number of RES evals.)
```

time	umax	k	nst	nni	nli	nre	nge	h	npe	nps
0.1000E-01	0.82411E+00	2	12	14	7	14+ 7	32	0.26E-02	8	21
0.2000E-01	0.68812E+00	3	15	18	12	18+12	32	0.51E-02	8	30
0.4000E-01	0.47093E+00	3	19	23	20	23+20	36	0.10E-01	9	43
0.8000E-01	0.21655E+00	3	23	27	32	27+32	36	0.10E-01	9	59
0.1600E+00	0.45225E-01	4	27	33	44	33+44	40	0.20E-01	10	77
0.3200E+00	0.21868E-02	3	34	41	67	41+67	44	0.41E-01	11	108
0.6400E+00	0.22218E-19	1	39	49	86	49+86	52	0.16E+00	13	135
0.1280E+01	0.19350E-19	1	41	51	86	51+86	60	0.66E+00	15	137

0.2560E+01	0.16748E-18	1	42	52	86	52+86	64	0.13E+01	16	138
0.5120E+01	0.13522E-17	1	43	53	86	53+86	68	0.26E+01	17	139
0.1024E+02	0.10274E-16	1	44	54	86	54+86	72	0.52E+01	18	140

Error test failures	=	0
Nonlinear convergence failures	=	0
Linear convergence failures	=	0

References

- [1] Peter N. Brown. Decay to uniform states in food webs. *SIAM J. Appl. Math.*, 46:376–392, 1986.
- [2] A. C. Hindmarsh and R. Serban. User Documentation for IDA v2.4.0. Technical Report UCRL-SM-208112, LLNL, 2005.
- [3] H. H. Robertson. The solution of a set of reaction rate equations. In J. Walsh, editor, *Numerical analysis: an introduction*, pages 178–182. Academ. Press, 1966.

A Listing of idadenx.c

```
1  /*
2  * -----
3  * $Revision: 1.4 $
4  * $Date: 2006/01/24 19:25:00 $
5  * -----
6  * Programmer(s): Allan Taylor, Alan Hindmarsh and
7  *                 Radu Serban @ LLNL
8  * -----
9  * This simple example problem for IDA, due to Robertson,
10 * is from chemical kinetics, and consists of the following three
11 * equations:
12 *
13 *     dy1/dt = -.04*y1 + 1.e4*y2*y3
14 *     dy2/dt = .04*y1 - 1.e4*y2*y3 - 3.e7*y2**2
15 *             0   = y1 + y2 + y3 - 1
16 *
17 * on the interval from t = 0.0 to t = 4.e10, with initial
18 * conditions: y1 = 1, y2 = y3 = 0.
19 *
20 * While integrating the system, we also use the rootfinding
21 * feature to find the points at which y1 = 1e-4 or at which
22 * y3 = 0.01.
23 *
24 * The problem is solved with IDA using IDADENSE for the linear
25 * solver, with a user-supplied Jacobian. Output is printed at
26 * t = .4, 4, 40, ..., 4e10.
27 * -----
28 */
29
30 #include <stdio.h>
31 #include <math.h>
32
33 #include "ida.h"
34 #include "nvector_serial.h"
35 #include "ida_dense.h"
36 #include "sundials_types.h"
37 #include "sundials_math.h"
38
39 /* Problem Constants */
40
41 #define NEQ    3
42 #define NOUT   12
43
44 #define ZERO  RCONST(0.0);
45 #define ONE   RCONST(1.0);
46
47 /* Macro to define dense matrix elements, indexed from 1. */
48
49 #define IJth(A,i,j) DENSE_ELEM(A,i-1,j-1)
50
51 /* Prototypes of functions called by IDA */
52
53 int resrob(realtype tres, N_Vector yy, N_Vector yp,
54             N_Vector resval, void *rdata);
55
56 static int grob(realtype t, N_Vector yy, N_Vector yp,
57                  realtype *gout, void *g_data);
```

```

58
59 int jacob(long int Neq, realtype tt, N_Vector yy, N_Vector yp,
60           N_Vector resvec, realtype cj, void *jdata, DenseMat JJ,
61           N_Vector tempv1, N_Vector tempv2, N_Vector tempv3);
62
63 /* Prototypes of private functions */
64 static void PrintHeader(realtype rtol, N_Vector avtol, N_Vector y);
65 static void PrintOutput(void *mem, realtype t, N_Vector y);
66 static void PrintRootInfo(int root_f1, int root_f2);
67 static void PrintFinalStats(void *mem);
68 static int check_flag(void *flagvalue, char *funcname, int opt);
69
70 /*
71 *-----*
72 * Main Program
73 *-----*/
74 */
75
76 int main(void)
77 {
78     void *mem;
79     N_Vector yy, yp, avtol;
80     realtype rtol, *yval, *ypval, *atval;
81     realtype t0, tout1, tout, tret;
82     int iout, retval, retvalr;
83     int rootsfound[2];
84
85     mem = NULL;
86     yy = yp = avtol = NULL;
87     yval = ypval = atval = NULL;
88
89     /* Allocate N-vectors. */
90     yy = N_VNew_Serial(NEQ);
91     if(check_flag((void *)yy, "N_VNew_Serial", 0)) return(1);
92     yp = N_VNew_Serial(NEQ);
93     if(check_flag((void *)yp, "N_VNew_Serial", 0)) return(1);
94     avtol = N_VNew_Serial(NEQ);
95     if(check_flag((void *)avtol, "N_VNew_Serial", 0)) return(1);
96
97     /* Create and initialize y, y', and absolute tolerance vectors. */
98     yval = NV_DATA_S(yy);
99     yval[0] = ONE;
100    yval[1] = ZERO;
101    yval[2] = ZERO;
102
103    ypval = NV_DATA_S(yp);
104    ypval[0] = RCONST(-0.04);
105    ypval[1] = RCONST(0.04);
106    ypval[2] = ZERO;
107
108    rtol = RCONST(1.0e-4);
109
110    atval = NV_DATA_S(avtol);
111    atval[0] = RCONST(1.0e-8);
112    atval[1] = RCONST(1.0e-14);
113    atval[2] = RCONST(1.0e-6);
114
115    /* Integration limits */
116    t0 = ZERO;

```

```

117 tout1 = RCONST(0.4);
118
119 PrintHeader(rtol, avtol, yy);
120
121 /* Call IDACreate and IDAMalloc to initialize IDA memory */
122 mem = IDACreate();
123 if(check_flag((void *)mem, "IDACreate", 0)) return(1);
124 retval = IDAMalloc(mem, resrob, t0, yy, yp, IDA_SV, rtol, avtol);
125 if(check_flag(&retval, "IDAMalloc", 1)) return(1);
126
127 /* Free avtol */
128 N_VDestroy_Serial(avtol);
129
130 /* Call IDARootInit to specify the root function grob with 2 components */
131 retval = IDARootInit(mem, 2, grob, NULL);
132 if (check_flag(&retval, "IDARootInit", 1)) return(1);
133
134 /* Call IDADense and set up the linear solver. */
135 retval = IDADense(mem, NEQ);
136 if(check_flag(&retval, "IDADense", 1)) return(1);
137 retval = IDADenseSetJacFn(mem, jacob, NULL);
138 if(check_flag(&retval, "IDADenseSetJacFn", 1)) return(1);
139
140 /* In loop, call IDASolve, print results, and test for error.
141      Break out of loop when NOUT preset output times have been reached. */
142
143 iout = 0; tout = tout1;
144 while(1) {
145
146     retval = IDASolve(mem, tout, &tret, yy, yp, IDA_NORMAL);
147
148     PrintOutput(mem,tret,yy);
149
150     if(check_flag(&retval, "IDASolve", 1)) return(1);
151
152     if (retval == IDA_ROOT_RETURN) {
153         retvalr = IDAGetRootInfo(mem, rootsfound);
154         check_flag(&retvalr, "IDAGetRootInfo", 1);
155         PrintRootInfo(rootsfound[0],rootsfound[1]);
156     }
157
158     if (retval == IDA_SUCCESS) {
159         iout++;
160         tout *= RCONST(10.0);
161     }
162
163     if (iout == NOUT) break;
164 }
165
166 PrintFinalStats(mem);
167
168 /* Free memory */
169
170 IDAFree(&mem);
171 N_VDestroy_Serial(yy);
172 N_VDestroy_Serial(yp);
173
174 return(0);
175

```

```

176 }
177
178 /*
179 *-----*
180 * Functions called by IDA
181 *-----*
182 */
183
184 /*
185 * Define the system residual function.
186 */
187
188 int resrob(realtype tres, N_Vector yy, N_Vector yp, N_Vector rr, void *rdata)
189 {
190     realtype *yval, *ypval, *rval;
191
192     yval = NV_DATA_S(yy);
193     ypval = NV_DATA_S(yp);
194     rval = NV_DATA_S(rr);
195
196     rval[0] = RCONST(-0.04)*yval[0] + RCONST(1.0e4)*yval[1]*yval[2];
197     rval[1] = -rval[0] - RCONST(3.0e7)*yval[1]*yval[1] - ypval[1];
198     rval[0] -= ypval[0];
199     rval[2] = yval[0] + yval[1] + yval[2] - ONE;
200
201     return(0);
202 }
203
204 /*
205 * Root function routine. Compute functions g_i(t,y) for i = 0,1.
206 */
207
208 static int grob(realtype t, N_Vector yy, N_Vector yp, realtype *gout,
209                  void *g_data)
210 {
211     realtype *yval, y1, y3;
212
213     yval = NV_DATA_S(yy);
214     y1 = yval[0]; y3 = yval[2];
215     gout[0] = y1 - RCONST(0.0001);
216     gout[1] = y3 - RCONST(0.01);
217
218     return(0);
219 }
220
221 /*
222 * Define the Jacobian function.
223 */
224
225 int jacrob(long int Neq, realtype tt, N_Vector yy, N_Vector yp,
226            N_Vector resvec, realtype cj, void *jdata, DenseMat JJ,
227            N_Vector tempv1, N_Vector tempv2, N_Vector tempv3)
228 {
229     realtype *yval;
230
231     yval = NV_DATA_S(yy);
232
233     IJth(JJ,1,1) = RCONST(-0.04) - cj;
234     IJth(JJ,2,1) = RCONST(0.04);

```

```

235     IJth(JJ,3,1) = ONE;
236     IJth(JJ,1,2) = RCONST(1.0e4)*yval[2];
237     IJth(JJ,2,2) = RCONST(-1.0e4)*yval[2] - RCONST(6.0e7)*yval[1] - cj;
238     IJth(JJ,3,2) = ONE;
239     IJth(JJ,1,3) = RCONST(1.0e4)*yval[1];
240     IJth(JJ,2,3) = RCONST(-1.0e4)*yval[1];
241     IJth(JJ,3,3) = ONE;
242
243     return(0);
244 }
245
246 /*
247 *-----
248 * Private functions
249 *-----
250 */
251
252 /*
253 * Print first lines of output (problem description)
254 */
255
256 static void PrintHeader(realtype rtol, N_Vector avtol, N_Vector y)
257 {
258     realtype *atval, *yval;
259
260     atval = NV_DATA_S(avtol);
261     yval = NV_DATA_S(y);
262
263     printf("\nidabenx: Robertson kinetics DAE serial example problem for IDA\n");
264     printf(" Three equation chemical kinetics problem.\n\n");
265     printf("Linear solver: IDADENSE, with user-supplied Jacobian.\n");
266 #if defined(SUNDIALS_EXTENDED_PRECISION)
267     printf("Tolerance parameters: rtol= %Lg atol= %Lg %Lg %Lg\n",
268            rtol, atval[0], atval[1], atval[2]);
269     printf("Initial conditions y0= (%Lg %Lg %Lg)\n",
270            yval[0], yval[1], yval[2]);
271 #elif defined(SUNDIALS_DOUBLE_PRECISION)
272     printf("Tolerance parameters: rtol= %lg atol= %lg %lg %lg\n",
273            rtol, atval[0], atval[1], atval[2]);
274     printf("Initial conditions y0= (%lg %lg %lg)\n",
275            yval[0], yval[1], yval[2]);
276 #else
277     printf("Tolerance parameters: rtol= %g atol= %g %g %g\n",
278            rtol, atval[0], atval[1], atval[2]);
279     printf("Initial conditions y0= (%g %g %g)\n",
280            yval[0], yval[1], yval[2]);
281 #endif
282     printf("Constraints and id not used.\n\n");
283     printf("-----\n");
284     printf(" ut | y1 | y2 | y3 ");
285     printf(" un | nst | k | h \n");
286     printf("-----\n");
287 }
288
289 /*
290 * Print Output
291 */
292
293 static void PrintOutput(void *mem, realtype t, N_Vector y)

```

```

294 {
295     realtype *yval;
296     int retval, kused;
297     long int nst;
298     realtype hused;
299
300     yval = NV_DATA_S(y);
301
302     retval = IDAGetLastOrder(mem, &kused);
303     check_flag(&retval, "IDAGetLastOrder", 1);
304     retval = IDAGetNumSteps(mem, &nst);
305     check_flag(&retval, "IDAGetNumSteps", 1);
306     retval = IDAGetLastStep(mem, &hused);
307     check_flag(&retval, "IDAGetLastStep", 1);
308 #if defined(SUNDIALS_EXTENDED_PRECISION)
309     printf("%10.4Le\u2022%12.4Le\u2022%12.4Le\u2022%3ld\u2022%1d\u2022%12.4Le\n",
310           t, yval[0], yval[1], yval[2], nst, kused, hused);
311 #elif defined(SUNDIALS_DOUBLE_PRECISION)
312     printf("%10.4le\u2022%12.4le\u2022%12.4le\u2022%3ld\u2022%1d\u2022%12.4le\n",
313           t, yval[0], yval[1], yval[2], nst, kused, hused);
314 #else
315     printf("%10.4e\u2022%12.4e\u2022%12.4e\u2022%3ld\u2022%1d\u2022%12.4e\n",
316           t, yval[0], yval[1], yval[2], nst, kused, hused);
317 #endif
318 }
319
320 static void PrintRootInfo(int root_f1, int root_f2)
321 {
322     printf("uuuurootsfound[]\u2022=%3d\u2022%3d\n", root_f1, root_f2);
323     return;
324 }
325
326 /*
327  * Print final integrator statistics
328 */
329
330 static void PrintFinalStats(void *mem)
331 {
332     int retval;
333     long int nst, nni, nje, nre, nreLS, netf, ncfn, nge;
334
335     retval = IDAGetNumSteps(mem, &nst);
336     check_flag(&retval, "IDAGetNumSteps", 1);
337     retval = IDAGetNumResEvals(mem, &nre);
338     check_flag(&retval, "IDAGetNumResEvals", 1);
339     retval = IDADenseGetNumJacEvals(mem, &nje);
340     check_flag(&retval, "IDADenseGetNumJacEvals", 1);
341     retval = IDAGetNumNonlinSolvIters(mem, &nni);
342     check_flag(&retval, "IDAGetNumNonlinSolvIters", 1);
343     retval = IDAGetNumErrTestFails(mem, &netf);
344     check_flag(&retval, "IDAGetNumErrTestFails", 1);
345     retval = IDAGetNumNonlinSolvConvFails(mem, &ncfn);
346     check_flag(&retval, "IDAGetNumNonlinSolvConvFails", 1);
347     retval = IDADenseGetNumResEvals(mem, &nreLS);
348     check_flag(&retval, "IDADenseGetNumResEvals", 1);
349     retval = IDAGetNumGEvals(mem, &nge);
350     check_flag(&retval, "IDAGetNumGEvals", 1);
351
352     printf("\nFinal\u2022Run\u2022Statistics:\u2022\n\n");

```

```

353 printf("Number of steps = %ld\n", nst);
354 printf("Number of residual evaluations = %ld\n", nre+nreLS);
355 printf("Number of Jacobian evaluations = %ld\n", nje);
356 printf("Number of nonlinear iterations = %ld\n", nni);
357 printf("Number of error test failures = %ld\n", netf);
358 printf("Number of nonlinear conv. failures = %ld\n", ncfn);
359 printf("Number of root fn. evaluations = %ld\n", nge);
360 }
361
362 /*
363 * Check function return value...
364 *   opt == 0 means SUNDIALS function allocates memory so check if
365 *           returned NULL pointer
366 *   opt == 1 means SUNDIALS function returns a flag so check if
367 *           flag >= 0
368 *   opt == 2 means function allocates memory so check if returned
369 *           NULL pointer
370 */
371
372 static int check_flag(void *flagvalue, char *funcname, int opt)
373 {
374     int *errflag;
375     /* Check if SUNDIALS function returned NULL pointer - no memory allocated */
376     if (opt == 0 && flagvalue == NULL) {
377         fprintf(stderr,
378                 "\nSUNDIALS_ERROR: %s() failed - returned NULL pointer\n\n",
379                 funcname);
380         return(1);
381     } else if (opt == 1) {
382         /* Check if flag < 0 */
383         errflag = (int *) flagvalue;
384         if (*errflag < 0) {
385             fprintf(stderr,
386                     "\nSUNDIALS_ERROR: %s() failed with flag = %d\n\n",
387                     funcname, *errflag);
388             return(1);
389         }
390     } else if (opt == 2 && flagvalue == NULL) {
391         /* Check if function returned NULL pointer - no memory allocated */
392         fprintf(stderr,
393                 "\nMEMORY_ERROR: %s() failed - returned NULL pointer\n\n",
394                 funcname);
395         return(1);
396     }
397
398     return(0);
399 }

```

B Listing of idabanx2.c

```

1  /*
2  * -----
3  * $Revision: 1.3 $
4  * $Date: 2006/03/17 16:58:00 $
5  * -----
6  * Programmer(s): Allan Taylor, Alan Hindmarsh and
7  *                 Radu Serban @ LLNL
8  * -----
9  * Example program for IDA: Food web problem.
10 *
11 * This example program (serial version) uses the IDABAND linear
12 * solver, and IDACalcIC for initial condition calculation.
13 *
14 * The mathematical problem solved in this example is a DAE system
15 * that arises from a system of partial differential equations after
16 * spatial discretization. The PDE system is a food web population
17 * model, with predator-prey interaction and diffusion on the unit
18 * square in two dimensions. The dependent variable vector is:
19 *
20 *      1   2           ns
21 *      c = (c , c , ... , c ) , ns = 2 * np
22 *
23 * and the PDE's are as follows:
24 *
25 *      i           i           i
26 *      dc /dt = d(i)*(c + c ) + R (x,y,c)   (i = 1,...,np)
27 *                  xx       yy           i
28 *
29 *      i           i
30 *      0 = d(i)*(c + c ) + R (x,y,c)   (i = np+1,...,ns)
31 *                  xx       yy           i
32 *
33 * where the reaction terms R are:
34 *
35 *      i           ns           j
36 *      R (x,y,c) = c * (b(i) + sum a(i,j)*c )
37 *                  i           j=1
38 *
39 * The number of species is ns = 2 * np, with the first np being
40 * prey and the last np being predators. The coefficients a(i,j),
41 * b(i), d(i) are:
42 *
43 * a(i,i) = -AA    (all i)
44 * a(i,j) = -GG    (i <= np , j > np)
45 * a(i,j) = EE    (i > np, j <= np)
46 * all other a(i,j) = 0
47 * b(i) = BB*(1+ alpha * x*y + beta*sin(4 pi x)*sin(4 pi y)) (i <= np)
48 * b(i) = -BB*(1+ alpha * x*y + beta*sin(4 pi x)*sin(4 pi y)) (i > np)
49 * d(i) = DPREY   (i <= np)
50 * d(i) = DPRED   (i > np)
51 *
52 * The various scalar parameters required are set using '#define'
53 * statements or directly in routine InitUserData. In this program,
54 * np = 1, ns = 2. The boundary conditions are homogeneous Neumann:
55 * normal derivative = 0.
56 *
57 * A polynomial in x and y is used to set the initial values of the

```

```

58 * first np variables (the prey variables) at each x,y location,
59 * while initial values for the remaining (predator) variables are
60 * set to a flat value, which is corrected by IDACalcIC.
61 *
62 * The PDEs are discretized by central differencing on a MX by MY
63 * mesh.
64 *
65 * The DAE system is solved by IDA using the IDABAND linear solver.
66 * Output is printed at t = 0, .001, .01, .1, .4, .7, 1.
67 * -----
68 * References:
69 * [1] Peter N. Brown and Alan C. Hindmarsh,
70 *      Reduced Storage Matrix Methods in Stiff ODE systems, Journal
71 *      of Applied Mathematics and Computation, Vol. 31 (May 1989),
72 *      pp. 40-91.
73 *
74 * [2] Peter N. Brown, Alan C. Hindmarsh, and Linda R. Petzold,
75 *      Using Krylov Methods in the Solution of Large-Scale
76 *      Differential-Algebraic Systems, SIAM J. Sci. Comput., 15
77 *      (1994), pp. 1467-1488.
78 *
79 * [3] Peter N. Brown, Alan C. Hindmarsh, and Linda R. Petzold,
80 *      Consistent Initial Condition Calculation for Differential-
81 *      Algebraic Systems, SIAM J. Sci. Comput., 19 (1998),
82 *      pp. 1495-1512.
83 * -----
84 */
85
86 #include <stdio.h>
87 #include <stdlib.h>
88 #include <math.h>
89
90 #include "ida.h"           /* Main header file */
91 #include "nvector_serial.h" /* Definitions of N_Vector and NV_DATA_S */
92 #include "ida_band.h"       /* Use IDABAND linear solver */
93 #include "sundials_smalldense.h" /* Definition of denalloc */
94 #include "sundials_types.h" /* Definitions of realtype and booleantype */
95
96 /* Problem Constants. */
97
98 #define NPREY      1           /* No. of prey (= no. of predators). */
99 #define NUM_SPECIES 2*NPREY
100
101 #define PI          RCONST(3.1415926535898)
102 #define FOURPI     (RCONST(4.0)*PI)
103
104 #define MX          20          /* MX = number of x mesh points */
105 #define MY          20          /* MY = number of y mesh points */
106 #define NSMX        (NUM_SPECIES * MX)
107 #define NEQ         (NUM_SPECIES*MX*MY)
108 #define AA          RCONST(1.0) /* Coefficient in above eqns. for a */
109 #define EE          RCONST(10000.) /* Coefficient in above eqns. for a */
110 #define GG          RCONST(0.5e-6) /* Coefficient in above eqns. for a */
111 #define BB          RCONST(1.0) /* Coefficient in above eqns. for b */
112 #define DPREY       RCONST(1.0) /* Coefficient in above eqns. for d */
113 #define DPRED       RCONST(0.05) /* Coefficient in above eqns. for d */
114 #define ALPHA       RCONST(50.) /* Coefficient alpha in above eqns. */
115 #define BETA        RCONST(1000.) /* Coefficient beta in above eqns. */
116 #define AX          RCONST(1.0) /* Total range of x variable */

```

```

117 #define AY RCONST(1.0) /* Total range of y variable */
118 #define RTOL RCONST(1.e-5) /* Relative tolerance */
119 #define ATOL RCONST(1.e-5) /* Absolute tolerance */
120 #define NOUT 6 /* Number of output times */
121 #define TMULT RCONST(10.0) /* Multiplier for tout values */
122 #define TADD RCONST(0.3) /* Increment for tout values */
123 #define ZERO RCONST(0.)
124 #define ONE RCONST(1.0)

125 /*
126 * User-defined vector and accessor macro: IJ_Vptr.
127 * IJ_Vptr is defined in order to express the underlying 3-D structure of
128 * the dependent variable vector from its underlying 1-D storage (an N_Vector).
129 * IJ_Vptr(vv,i,j) returns a pointer to the location in vv corresponding to
130 * species index is = 0, x-index ix = i, and y-index jy = j.
131 */
132 */

133
134 #define IJ_Vptr(vv,i,j) (&NV_Ith_S(vv, (i)*NUM_SPECIES + (j)*NSMX))
135
136 /* Type: UserData. Contains problem constants, etc. */
137
138 typedef struct {
139     long int Neq, ns, np, mx, my;
140     realtype dx, dy, **acoef;
141     realtype cox[NUM_SPECIES], coy[NUM_SPECIES], bcoef[NUM_SPECIES];
142     N_Vector rates;
143 } *UserData;
144
145 /* Prototypes for functions called by the IDA Solver. */
146
147 static int resweb(realtype time, N_Vector cc, N_Vector cp, N_Vector resval,
148                   void *rdata);
149
150 /* Prototypes for private Helper Functions. */
151
152 static void InitUserData(UserData webdata);
153 static void SetInitialProfiles(N_Vector cc, N_Vector cp, N_Vector id,
154                               UserData webdata);
155 static void PrintHeader(long int mu, long int ml, realtype rtol, realtype atol);
156 static void PrintOutput(void *mem, N_Vector c, realtype t);
157 static void PrintFinalStats(void *mem);
158 static void Fweb(realtype tcalc, N_Vector cc, N_Vector crate, UserData webdata);
159 static void WebRates(realtype xx, realtype yy, realtype *cxy, realtype *ratesxy,
160                      UserData webdata);
161 static realtype dotprod(long int size, realtype *x1, realtype *x2);
162 static int check_flag(void *flagvalue, char *funcname, int opt);
163
164 /*
165 *-----*
166 * MAIN PROGRAM
167 *-----*
168 */
169
170 int main()
171 {
172     void *mem;
173     UserData webdata;
174     N_Vector cc, cp, id;
175     int iout, retval;

```

```

176 long int mu, ml;
177 realtype rtol, atol, t0, tout, tret;
178
179 mem = NULL;
180 webdata = NULL;
181 cc = cp = id = NULL;
182
183 /* Allocate and initialize user data block webdata. */
184
185 webdata = (UserData) malloc(sizeof *webdata);
186 webdata->rates = N_VNew_Serial(NEQ);
187 webdata->acoef = denalloc(NUM_SPECIES);
188
189 InitUserData(webdata);
190
191 /* Allocate N-vectors and initialize cc, cp, and id. */
192
193 cc = N_VNew_Serial(NEQ);
194 if(check_flag((void *)cc, "N_VNew_Serial", 0)) return(1);
195
196 cp = N_VNew_Serial(NEQ);
197 if(check_flag((void *)cp, "N_VNew_Serial", 0)) return(1);
198
199 id = N_VNew_Serial(NEQ);
200 if(check_flag((void *)id, "N_VNew_Serial", 0)) return(1);
201
202 SetInitialProfiles(cc, cp, id, webdata);
203
204 /* Set remaining inputs to IDAMalloc. */
205
206 t0 = ZERO;
207 rtol = RTOL;
208 atol = ATOL;
209
210 /* Call IDACreate and IDAMalloc to initialize IDA. */
211
212 mem = IDACreate();
213 if(check_flag((void *)mem, "IDACreate", 0)) return(1);
214
215 retval = IDASetRdata(mem, webdata);
216 if(check_flag(&retval, "IDASetRdata", 1)) return(1);
217
218 retval = IDASetId(mem, id);
219 if(check_flag(&retval, "IDASetId", 1)) return(1);
220
221 retval = IDAMalloc(mem, resweb, t0, cc, cp, IDA_SS, rtol, &atol);
222 if(check_flag(&retval, "IDAMalloc", 1)) return(1);
223
224 /* Call IDABand to specify the IDA linear solver. */
225
226 mu = ml = NSMX;
227 retval = IDABand(mem, NEQ, mu, ml);
228 if(check_flag(&retval, "IDABand", 1)) return(1);
229
230 /* Call IDACalcIC (with default options) to correct the initial values. */
231
232 tout = RCONST(0.001);
233 retval = IDACalcIC(mem, t0, cc, cp, IDA_YA_YDP_INIT, tout);
234 if(check_flag(&retval, "IDACalcIC", 1)) return(1);

```

```

235
236     /* Print heading, basic parameters, and initial values. */
237
238     PrintHeader(mu, ml, rtol, atol);
239     PrintOutput(mem, cc, ZERO);
240
241     /* Loop over iout, call IDASolve (normal mode), print selected output. */
242
243     for (iout = 1; iout <= NOUT; iout++) {
244
245         retval = IDASolve(mem, tout, &tret, cc, cp, IDA_NORMAL);
246         if(check_flag(&retval, "IDASolve", 1)) return(retval);
247
248         PrintOutput(mem, cc, tret);
249
250         if (iout < 3) tout *= TMULT; else tout += TADD;
251
252     }
253
254     /* Print final statistics and free memory. */
255
256     PrintFinalStats(mem);
257
258     /* Free memory */
259
260     IDAFree(&mem);
261
262     N_VDestroy_Serial(cc);
263     N_VDestroy_Serial(cp);
264     N_VDestroy_Serial(id);
265
266
267     denfree(webdata->acoef);
268     N_VDestroy_Serial(webdata->rates);
269     free(webdata);
270
271     return(0);
272 }
273
274 /* Define lines for readability in later routines */
275
276 #define acoef (webdata->acoef)
277 #define bcoef (webdata->bcoef)
278 #define cox (webdata->cox)
279 #define coy (webdata->coy)
280
281 /*
282 *-----*
283 * FUNCTIONS CALLED BY IDA
284 *-----*
285 */
286
287 /*
288 * resweb: System residual function for predator-prey system.
289 * This routine calls Fweb to get all the right-hand sides of the
290 * equations, then loads the residual vector accordingly,
291 * using cp in the case of prey species.
292 */
293

```

```

294 static int resweb(realtype tt, N_Vector cc, N_Vector cp,
295                     N_Vector res, void *rdata)
296 {
297     long int jx, jy, is, yloc, loc, np;
298     realtype *resv, *cpv;
299     UserData webdata;
300
301     webdata = (UserData)rdata;
302
303     cpv = NV_DATA_S(cp);
304     resv = NV_DATA_S(res);
305     np = webdata->np;
306
307     /* Call Fweb to set res to vector of right-hand sides. */
308     Fweb(tt, cc, res, webdata);
309
310     /* Loop over all grid points, setting residual values appropriately
311      for differential or algebraic components. */
```

312
313 for (jy = 0; jy < MY; jy++) {
314 yloc = NSMX * jy;
315 for (jx = 0; jx < MX; jx++) {
316 loc = yloc + NUM_SPECIES * jx;
317 for (is = 0; is < NUM_SPECIES; is++) {
318 if (is < np)
319 resv[loc+is] = cpv[loc+is] - resv[loc+is];
320 else
321 resv[loc+is] = -resv[loc+is];
322 }
323 }
324 }
325
326 return(0);
327 }
328
329 /*
330 *-----*
331 * PRIVATE FUNCTIONS
332 *-----*
333 */
334
335
336 /*
337 * InitUserData: Load problem constants in webdata (of type UserData).
338 */
339
340 static void InitUserData(UserData webdata)
341 {
342 int i, j, np;
343 realtype *a1,*a2, *a3, *a4, dx2, dy2;
344
345 webdata->mx = MX;
346 webdata->my = MY;
347 webdata->ns = NUM_SPECIES;
348 webdata->np = NPREY;
349 webdata->dx = AX/(MX-1);
350 webdata->dy = AY/(MY-1);
351 webdata->Neq= NEQ;
352 }

```

353 /* Set up the coefficients a and b, and others found in the equations. */
354 np = webdata->np;
355 dx2 = (webdata->dx)*(webdata->dx); dy2 = (webdata->dy)*(webdata->dy);
356
357 for (i = 0; i < np; i++) {
358     a1 = &(acoef[i][np]);
359     a2 = &(acoef[i+np][0]);
360     a3 = &(acoef[i][0]);
361     a4 = &(acoef[i+np][np]);
362     /* Fill in the portion of acoef in the four quadrants, row by row. */
363     for (j = 0; j < np; j++) {
364         *a1++ = -GG;
365         *a2++ = EE;
366         *a3++ = ZERO;
367         *a4++ = ZERO;
368     }
369
370     /* Reset the diagonal elements of acoef to -AA. */
371     acoef[i][i] = -AA; acoef[i+np][i+np] = -AA;
372
373     /* Set coefficients for b and diffusion terms. */
374     bcoef[i] = BB; bcoef[i+np] = -BB;
375     cox[i] = DPREY/dx2; cox[i+np] = DPRED/dx2;
376     coy[i] = DPREY/dy2; coy[i+np] = DPRED/dy2;
377 }
378
379 }
380
381 /*
382 * SetInitialProfiles: Set initial conditions in cc, cp, and id.
383 * A polynomial profile is used for the prey cc values, and a constant
384 * (1.0e5) is loaded as the initial guess for the predator cc values.
385 * The id values are set to 1 for the prey and 0 for the predators.
386 * The prey cp values are set according to the given system, and
387 * the predator cp values are set to zero.
388 */
389
390 static void SetInitialProfiles(N_Vector cc, N_Vector cp, N_Vector id,
391                             UserData webdata)
392 {
393     long int loc, yloc, is, jx, jy, np;
394     realtype xx, yy, xyfactor, fac;
395     realtype *ccv, *cpv, *idv;
396
397     ccv = NV_DATA_S(cc);
398     cpv = NV_DATA_S(cp);
399     idv = NV_DATA_S(id);
400     np = webdata->np;
401
402     /* Loop over grid, load cc values and id values. */
403     for (jy = 0; jy < MY; jy++) {
404         yy = jy * webdata->dy;
405         yloc = NSMX * jy;
406         for (jx = 0; jx < MX; jx++) {
407             xx = jx * webdata->dx;
408             xyfactor = RCONST(16.0)*xx*(ONE-xx)*yy*(ONE-yy);
409             xyfactor *= xyfactor;
410             loc = yloc + NUM_SPECIES*jx;
411             fac = ONE + ALPHA * xx * yy + BETA * sin(FOURPI*xx) * sin(FOURPI*yy);

```

```

412
413     for (is = 0; is < NUM_SPECIES; is++) {
414         if (is < np) {
415             ccv[loc+is] = RCONST(10.0) + (realtype)(is+1) * xyfactor;
416             idv[loc+is] = ONE;
417         }
418         else {
419             ccv[loc+is] = RCONST(1.0e5);
420             idv[loc+is] = ZERO;
421         }
422     }
423 }
424 }

425 /* Set c' for the prey by calling the function Fweb. */
426 Fweb(ZERO, cc, cp, webdata);
427

428 /* Set c' for predators to 0. */
429 for (jy = 0; jy < MY; jy++) {
430     yloc = NSMX * jy;
431     for (jx = 0; jx < MX; jx++) {
432         loc = yloc + NUM_SPECIES * jx;
433         for (is = np; is < NUM_SPECIES; is++) {
434             cpv[loc+is] = ZERO;
435         }
436     }
437 }
438 }

439 */

440 /*
441 * Print first lines of output (problem description)
442 */
443

444 static void PrintHeader(long int mu, long int ml, realtype rtol, realtype atol)
445 {
446     printf("\nidabanx2: Predator-prey DAE serial example problem for IDA\n\n");
447     printf("Number of species: %d", NUM_SPECIES);
448     printf(" Mesh dimensions: %d x %d", MX, MY);
449     printf(" System size: %d\n", NEQ);
450 #if defined(SUNDIALS_EXTENDED_PRECISION)
451     printf("Tolerance parameters: rtol=%Lg, atol=%Lg\n", rtol, atol);
452 #elif defined(SUNDIALS_DOUBLE_PRECISION)
453     printf("Tolerance parameters: rtol=%lg, atol=%lg\n", rtol, atol);
454 #else
455     printf("Tolerance parameters: rtol=%g, atol=%g\n", rtol, atol);
456 #endif
457     printf("Linear solver: IDABAND, Band parameters mu= %ld, ml= %ld\n", mu, ml);
458     printf("CalcIC called to correct initial predator concentrations.\n\n");
459     printf("-----\n");
460     printf(" bottom-left top-right");
461     printf(" | nstukh\n");
462     printf("-----\n\n");
463 }

464 */

465 /*
466 * PrintOutput: Print output values at output time t = tt.
467 * Selected run statistics are printed. Then values of the concentrations
468 * are printed for the bottom left and top right grid points only.

```

```

471     */
472
473 static void PrintOutput(void *mem, N_Vector c, realtype t)
474 {
475     int i, kused, flag;
476     long int nst;
477     realtype *c_b1, *c_tr, hused;
478
479     flag = IDAGetLastOrder(mem, &kused);
480     check_flag(&flag, "IDAGetLastOrder", 1);
481     flag = IDAGetNumSteps(mem, &nst);
482     check_flag(&flag, "IDAGetNumSteps", 1);
483     flag = IDAGetLastStep(mem, &hused);
484     check_flag(&flag, "IDAGetLastStep", 1);
485
486     c_b1 = IJ_Vptr(c, 0, 0);
487     c_tr = IJ_Vptr(c, MX-1, MY-1);
488
489 #if defined(SUNDIALS_EXTENDED_PRECISION)
490     printf("%8.2Le%12.4Le%12.4Leuuu|u%3lduu%1d%12.4Le\n",
491            t, c_b1[0], c_tr[1], nst, kused, hused);
492     for (i=1;i<NUM_SPECIES;i++)
493         printf("uuuuuuuuuu%12.4Le%12.4Leuuu|\n", c_b1[i], c_tr[i]);
494 #elif defined(SUNDIALS_DOUBLE_PRECISION)
495     printf("%8.2le%12.4le%12.4leuuu|u%3lduu%1d%12.4le\n",
496            t, c_b1[0], c_tr[1], nst, kused, hused);
497     for (i=1;i<NUM_SPECIES;i++)
498         printf("uuuuuuuuuu%12.4le%12.4leuuu|\n", c_b1[i], c_tr[i]);
499 #else
500     printf("%8.2e%12.4e%12.4euuu|u%3lduu%1d%12.4e\n",
501            t, c_b1[0], c_tr[1], nst, kused, hused);
502     for (i=1;i<NUM_SPECIES;i++)
503         printf("uuuuuuuuuu%12.4e%12.4euuu|\n", c_b1[i], c_tr[i]);
504 #endif
505
506     printf("\n");
507 }
508
509 /*
510  * PrintFinalStats: Print final run data contained in iopt.
511  */
512
513 static void PrintFinalStats(void *mem)
514 {
515     long int nst, nre, nreLS, nni, nje, netf, ncfn;
516     int flag;
517
518     flag = IDAGetNumSteps(mem, &nst);
519     check_flag(&flag, "IDAGetNumSteps", 1);
520     flag = IDAGetNumNonlinSolvIterers(mem, &nni);
521     check_flag(&flag, "IDAGetNumNonlinSolvIterers", 1);
522     flag = IDAGetNumResEvals(mem, &nre);
523     check_flag(&flag, "IDAGetNumResEvals", 1);
524     flag = IDAGetNumErrTestFails(mem, &netf);
525     check_flag(&flag, "IDAGetNumErrTestFails", 1);
526     flag = IDAGetNumNonlinSolvConvFails(mem, &ncfn);
527     check_flag(&flag, "IDAGetNumNonlinSolvConvFails", 1);
528     flag = IDABandGetNumJacEvals(mem, &nje);
529     check_flag(&flag, "IDABandGetNumJacEvals", 1);

```

```

530 flag = IDABandGetNumResEvals(mem, &nreLS);
531 check_flag(&flag, "IDABandGetNumResEvals", 1);
532
533 printf("-----\n");
534 printf("Final run statistics:\n");
535 printf("Number of steps = %ld\n", nst);
536 printf("Number of residual evaluations = %ld\n", nre+nreLS);
537 printf("Number of Jacobian evaluations = %ld\n", nje);
538 printf("Number of nonlinear iterations = %ld\n", nni);
539 printf("Number of error test failures = %ld\n", netf);
540 printf("Number of nonlinear conv. failures = %ld\n", ncfn);
541
542 }
543
544 /*
545 * Fweb: Rate function for the food-web problem.
546 * This routine computes the right-hand sides of the system equations,
547 * consisting of the diffusion term and interaction term.
548 * The interaction term is computed by the function WebRates.
549 */
550
551 static void Fweb(realtyp tcalc, N_Vector cc, N_Vector crate,
552 Userdata webdata)
553 {
554 long int jx, jy, is, idyu, idyl, idxu, idxl;
555 realtyp xx, yy, *cxy, *ratesxy, *cratexy, dcyli, dcyui, dcxli, dcxui;
556
557 /* Loop over grid points, evaluate interaction vector (length ns),
558 form diffusion difference terms, and load crate. */
559
560 for (jy = 0; jy < MY; jy++) {
561 yy = (webdata->dy) * jy ;
562 idyu = (jy!=MY-1) ? NSMX : -NSMX;
563 idyl = (jy!= 0 ) ? NSMX : -NSMX;
564
565 for (jx = 0; jx < MX; jx++) {
566 xx = (webdata->dx) * jx;
567 idxu = (jx!= MX-1) ? NUM_SPECIES : -NUM_SPECIES;
568 idxl = (jx!= 0 ) ? NUM_SPECIES : -NUM_SPECIES;
569 cxy = IJ_Vptr(cc,jx,jy);
570 ratesxy = IJ_Vptr(webdata->rates,jx,jy);
571 cratexy = IJ_Vptr(crate,jx,jy);
572
573 /* Get interaction vector at this grid point. */
574 WebRates(xx, yy, cxy, ratesxy, webdata);
575
576 /* Loop over species, do differencing, load crate segment. */
577 for (is = 0; is < NUM_SPECIES; is++) {
578
579 /* Differencing in y. */
580 dcyli = *(cxy+is) - *(cxy - idyl + is) ;
581 dcyui = *(cxy + idyu + is) - *(cxy+is);
582
583 /* Differencing in x. */
584 dcxli = *(cxy+is) - *(cxy - idxl + is);
585 dcxui = *(cxy + idxu + is) - *(cxy+is);
586
587 /* Compute the crate values at (xx,yy). */
588 cratexy[is] = coy[is] * (dcyui - dcyli) +

```

```

589         cox[is] * (dcxui - dcxli) + ratesxy[is];
590
591     } /* End is loop */
592 } /* End of jx loop */
593 } /* End of jy loop */
594
595 }
596
597 /*
598 * WebRates: Evaluate reaction rates at a given spatial point.
599 * At a given (x,y), evaluate the array of ns reaction terms R.
600 */
601
602 static void WebRates(realtype xx, realtype yy, realtype *cxy, realtype *ratesxy,
603                      UserData webdata)
604 {
605     int is;
606     realtype fac;
607
608     for (is = 0; is < NUM_SPECIES; is++)
609         ratesxy[is] = dotprod(NUM_SPECIES, cxy, acoef[is]);
610
611     fac = ONE + ALPHA*xx*yy + BETA*sin(FOURPI*xx)*sin(FOURPI*yy);
612
613     for (is = 0; is < NUM_SPECIES; is++)
614         ratesxy[is] = cxy[is]*( bcoef[is]*fac + ratesxy[is] );
615
616 }
617
618 /*
619 * dotprod: dot product routine for realtype arrays, for use by WebRates.
620 */
621
622 static realtype dotprod(long int size, realtype *x1, realtype *x2)
623 {
624     long int i;
625     realtype *xx1, *xx2, temp = ZERO;
626
627     xx1 = x1; xx2 = x2;
628     for (i = 0; i < size; i++) temp += (*xx1++) * (*xx2++);
629     return(temp);
630
631 }
632
633 /*
634 * Check function return value...
635 *   opt == 0 means SUNDIALS function allocates memory so check if
636 *           returned NULL pointer
637 *   opt == 1 means SUNDIALS function returns a flag so check if
638 *           flag >= 0
639 *   opt == 2 means function allocates memory so check if returned
640 *           NULL pointer
641 */
642
643 static int check_flag(void *flagvalue, char *funcname, int opt)
644 {
645     int *errflag;
646
647     if (opt == 0 && flagvalue == NULL) {

```

```

648     /* Check if SUNDIALS function returned NULL pointer - no memory allocated */
649     fprintf(stderr,
650             "\nSUNDIALS_ERROR: %s() failed - returned NULL pointer\n\n",
651             funcname);
652     return(1);
653 } else if (opt == 1) {
654     /* Check if flag < 0 */
655     errflag = (int *) flagvalue;
656     if (*errflag < 0) {
657         fprintf(stderr,
658                 "\nSUNDIALS_ERROR: %s() failed with flag=%d\n\n",
659                 funcname, *errflag);
660         return(1);
661     }
662 } else if (opt == 2 && flagvalue == NULL) {
663     /* Check if function returned NULL pointer - no memory allocated */
664     fprintf(stderr,
665             "\nMEMORY_ERROR: %s() failed - returned NULL pointer\n\n",
666             funcname);
667     return(1);
668 }
669     return(0);
670 }

```

C Listing of idakryx.c

```
1  /*
2  * -----
3  * $Revision: 1.3 $
4  * $Date: 2006/02/02 00:34:28 $
5  * -----
6  * Programmer(s): Allan Taylor, Alan Hindmarsh and
7  *                 Radu Serban @ LLNL
8  * -----
9  * Example problem for IDA: 2D heat equation, serial, GMRES.
10 *
11 * This example solves a discretized 2D heat equation problem.
12 * This version uses the Krylov solver IDASpgmr.
13 *
14 * The DAE system solved is a spatial discretization of the PDE
15 *      du/dt = d^2u/dx^2 + d^2u/dy^2
16 * on the unit square. The boundary condition is u = 0 on all edges.
17 * Initial conditions are given by u = 16 x (1 - x) y (1 - y). The
18 * PDE is treated with central differences on a uniform M x M grid.
19 * The values of u at the interior points satisfy ODEs, and
20 * equations u = 0 at the boundaries are appended, to form a DAE
21 * system of size N = M^2. Here M = 10.
22 *
23 * The system is solved with IDA/IDAS using the Krylov linear solver
24 * IDASPGMR. The preconditioner uses the diagonal elements of the
25 * Jacobian only. Routines for preconditioning, required by
26 * IDASPGMR, are supplied here. The constraints u >= 0 are posed
27 * for all components. Output is taken at t = 0, .01, .02, .04,
28 * ..., 10.24. Two cases are run -- with the Gram-Schmidt type
29 * being Modified in the first case, and Classical in the second.
30 * The second run uses IDAReInit and IDAReInitSpgmr.
31 *
32 */
33
34 #include <stdio.h>
35 #include <stdlib.h>
36 #include <math.h>
37
38 #include "ida.h"
39 #include "nvector_serial.h"
40 #include "ida_spgmr.h"
41 #include "sundials_types.h"
42
43 /* Problem Constants */
44
45 #define NOUT 11
46 #define MGRID 10
47 #define NEQ MGRID*MGRID
48 #define ZERO RCONST(0.0)
49 #define ONE RCONST(1.0)
50 #define TWO RCONST(2.0)
51 #define FOUR RCONST(4.0)
52
53 /* User data type */
54
55 typedef struct {
56     long int mm; /* number of grid points */
57     realtype dx;
```

```

58     realtype coeff;
59     N_Vecor pp; /* vector of prec. diag. elements */
60 } *UserData;
61
62 /* Prototypes for functions called by IDA */
63
64 int resHeat(realtype tres, N_Vecor uu, N_Vecor up,
65             N_Vecor resval, void *rdata);
66
67 int PsetupHeat(realtype tt,
68                 N_Vecor uu, N_Vecor up, N_Vecor rr,
69                 realtype c_j, void *prec_data,
70                 N_Vecor tmp1, N_Vecor tmp2, N_Vecor tmp3);
71
72 int PsolveHeat(realtype tt,
73                  N_Vecor uu, N_Vecor up, N_Vecor rr,
74                  N_Vecor rvec, N_Vecor zvec,
75                  realtype c_j, realtype delta, void *prec_data,
76                  N_Vecor tmp);
77
78 /* Prototypes for private functions */
79
80 static int SetInitialProfile(UserData data, N_Vecor uu, N_Vecor up,
81                             N_Vecor res);
82 static void PrintHeader(realtype rtol, realtype atol);
83 static void PrintOutput(void *mem, realtype t, N_Vecor uu);
84 static int check_flag(void *flagvalue, char *funcname, int opt);
85
86 /*
87 *-----*
88 * MAIN PROGRAM
89 *-----*
90 */
91
92 int main()
93 {
94     void *mem;
95     UserData data;
96     N_Vecor uu, up, constraints, res;
97     int ier, iout;
98     realtype rtol, atol, t0, t1, tout, tret;
99     long int netf, ncfn, ncfl;
100
101     mem = NULL;
102     data = NULL;
103     uu = up = constraints = res = NULL;
104
105     /* Allocate N-vectors and the user data structure. */
106
107     uu = N_VNew_Serial(NEQ);
108     if(check_flag((void *)uu, "N_VNew_Serial", 0)) return(1);
109
110     up = N_VNew_Serial(NEQ);
111     if(check_flag((void *)up, "N_VNew_Serial", 0)) return(1);
112
113     res = N_VNew_Serial(NEQ);
114     if(check_flag((void *)res, "N_VNew_Serial", 0)) return(1);
115
116     constraints = N_VNew_Serial(NEQ);

```

```

117 if(check_flag((void *)constraints, "N_VNew_Serial", 0)) return(1);
118
119 data = (UserData) malloc(sizeof *data);
120 data->pp = NULL;
121 if(check_flag((void *)data, "malloc", 2)) return(1);
122
123 /* Assign parameters in the user data structure. */
124
125 data->mm = MGRID;
126 data->dx = ONE/(MGRID-ONE);
127 data->coeff = ONE/(data->dx * data->dx);
128 data->pp = N_VNew_Serial(NEQ);
129 if(check_flag((void *)data->pp, "N_VNew_Serial", 0)) return(1);
130
131 /* Initialize uu, up. */
132
133 SetInitialProfile(data, uu, up, res);
134
135 /* Set constraints to all 1's for nonnegative solution values. */
136
137 N_VConst(ONE, constraints);
138
139 /* Assign various parameters. */
140
141 t0 = ZERO;
142 t1 = RCONST(0.01);
143 rtol = ZERO;
144 atol = RCONST(1.0e-3);
145
146 /* Call IDACreate and IDAMalloc to initialize solution */
147
148 mem = IDACreate();
149 if(check_flag((void *)mem, "IDACreate", 0)) return(1);
150
151 ier = IDASetRdata(mem, data);
152 if(check_flag(&ier, "IDASetRdata", 1)) return(1);
153
154 ier = IDASetConstraints(mem, constraints);
155 if(check_flag(&ier, "IDASetConstraints", 1)) return(1);
156 N_VDestroy_Serial(constraints);
157
158 ier = IDAMalloc(mem, resHeat, t0, uu, up, IDA_SS, rtol, &atol);
159 if(check_flag(&ier, "IDAMalloc", 1)) return(1);
160
161 /* Call IDASpgmr to specify the linear solver. */
162
163 ier = IDASpgmr(mem, 0);
164 if(check_flag(&ier, "IDASpgmr", 1)) return(1);
165
166 ier = IDASpilsSetPreconditioner(mem, PsetupHeat, PsolveHeat, data);
167 if(check_flag(&ier, "IDASpilsSetPreconditioner", 1)) return(1);
168
169 /* Print output heading. */
170 PrintHeader(rtol, atol);
171
172 /*
173 * -----
174 * CASE I
175 * -----

```

```

176   */
177
178 /* Print case number, output table heading, and initial line of table. */
179
180 printf("\n\nCase_1: gsytype=MODIFIED_GS\n");
181 printf("\nOutput_Summary_(umax_=max-norm_of_solution)\n\n");
182 printf("time umax knst nni nje nre nreLS huuuuu npe nps\n");
183 printf("-----\n");
184
185 /* Loop over output times, call IDASolve, and print results. */
186
187 for (tout = t1, iout = 1; iout <= NOUT ; iout++, tout *= TWO) {
188     ier = IDASolve(mem, tout, &tret, uu, up, IDA_NORMAL);
189     if(check_flag(&ier, "IDASolve", 1)) return(1);
190     PrintOutput(mem, tret, uu);
191 }
192
193 /* Print remaining counters. */
194
195 ier = IDAGetNumErrTestFails(mem, &netf);
196 check_flag(&ier, "IDAGetNumErrTestFails", 1);
197
198 ier = IDAGetNumNonlinSolvConvFails(mem, &ncfn);
199 check_flag(&ier, "IDAGetNumNonlinSolvConvFails", 1);
200
201 ier = IDASpilsGetNumConvFails(mem, &ncfl);
202 check_flag(&ier, "IDASpilsGetNumConvFails", 1);
203
204 printf("\nError test failures = %ld\n", netf);
205 printf("Nonlinear convergence failures = %ld\n", ncfn);
206 printf("Linear convergence failures = %ld\n", ncfl);
207
208 /*
209 * -----
210 * CASE II
211 * -----
212 */
213
214 /* Re-initialize uu, up. */
215
216 SetInitialProfile(data, uu, up, res);
217
218 /* Re-initialize IDA and IDASPGMR */
219
220 ier = IDAReInit(mem, resHeat, t0, uu, up, IDA_SS, rtol, &atol);
221 if(check_flag(&ier, "IDAReInit", 1)) return(1);
222
223 ier = IDASpilsSetGSType(mem, CLASSICAL_GS);
224 if(check_flag(&ier, "IDASpilsSetGSType", 1)) return(1);
225
226 /* Print case number, output table heading, and initial line of table. */
227
228 printf("\n\nCase_2: gsytype=CLASSICAL_GS\n");
229 printf("\nOutput_Summary_(umax_=max-norm_of_solution)\n\n");
230 printf("time umax knst nni nje nre nreLS huuuuu npe nps\n");
231 printf("-----\n");
232
233 /* Loop over output times, call IDASolve, and print results. */
234

```



```

294     up_data = NV_DATA_S(up);
295     rr_data = NV_DATA_S(rr);
296
297     data = (UserData) res_data;
298
299     coeff = data->coeff;
300     mm = data->mm;
301
302     /* Initialize rr to uu, to take care of boundary equations. */
303     N_VScale(ONE, uu, rr);
304
305     /* Loop over interior points; set res = up - (central difference). */
306     for (j = 1; j < MGRID-1; j++) {
307         offset = mm*j;
308         for (i = 1; i < mm-1; i++) {
309             loc = offset + i;
310             dif1 = uu_data[loc-1] + uu_data[loc+1] - TWO * uu_data[loc];
311             dif2 = uu_data[loc-mm] + uu_data[loc+mm] - TWO * uu_data[loc];
312             rr_data[loc] = up_data[loc] - coeff * (dif1 + dif2 );
313         }
314     }
315
316     return(0);
317 }
318
319 /*
320 * PsetupHeat: setup for diagonal preconditioner for idakryx.
321 *
322 * The optional user-supplied functions PsetupHeat and
323 * PsolveHeat together must define the left preconditioner
324 * matrix P approximating the system Jacobian matrix
325 *           J = dF/du + cj*dF/du'
326 * (where the DAE system is F(t,u,u') = 0), and solve the linear
327 * systems P z = r. This is done in this case by keeping only
328 * the diagonal elements of the J matrix above, storing them as
329 * inverses in a vector pp, when computed in PsetupHeat, for
330 * subsequent use in PsolveHeat.
331 *
332 * In this instance, only cj and data (user data structure, with
333 * pp etc.) are used from the PsetupdHeat argument list.
334 */
335
336 int PsetupHeat(realtype tt,
337                 N_Vector uu, N_Vector up, N_Vector rr,
338                 realtype c_j, void *prec_data,
339                 N_Vector tmp1, N_Vector tmp2, N_Vector tmp3)
340 {
341
342     long int i, j, offset, loc, mm;
343     realtype *ppv, pelinv;
344     UserData data;
345
346     data = (UserData) prec_data;
347     ppv = NV_DATA_S(data->pp);
348     mm = data->mm;
349
350     /* Initialize the entire vector to 1., then set the interior points to the
351      correct value for preconditioning. */
352     N_VConst(ONE,data->pp);

```

```

353
354     /* Compute the inverse of the preconditioner diagonal elements. */
355     pelinv = ONE/(c_j + FOUR*data->coeff);
356
357     for (j = 1; j < mm-1; j++) {
358         offset = mm * j;
359         for (i = 1; i < mm-1; i++) {
360             loc = offset + i;
361             ppv[loc] = pelinv;
362         }
363     }
364
365     return(0);
366 }
367
368 /*
369  * PsolveHeat: solve preconditioner linear system.
370  * This routine multiplies the input vector rvec by the vector pp
371  * containing the inverse diagonal Jacobian elements (previously
372  * computed in PrecondHeateq), returning the result in zvec.
373 */
374
375 int PsolveHeat(realtype tt,
376                 N_Vecor uu, N_Vecor up, N_Vecor rr,
377                 N_Vecor rvec, N_Vecor zvec,
378                 realtype c_j, realtype delta, void *prec_data,
379                 N_Vecor tmp)
380 {
381     UserData data;
382     data = (UserData) prec_data;
383     N_VProd(data->pp, rvec, zvec);
384     return(0);
385 }
386
387 /*
388 *-----*
389 * PRIVATE FUNCTIONS
390 *-----*
391 */
392
393 /*
394  * SetInitialProfile: routine to initialize u and up vectors.
395 */
396
397 static int SetInitialProfile(UserData data, N_Vecor uu, N_Vecor up,
398                             N_Vecor res)
399 {
400     long int mm, mm1, i, j, offset, loc;
401     realtype xfact, yfact, *udata, *updata;
402
403     mm = data->mm;
404
405     udata = NV_DATA_S(uu);
406     updata = NV_DATA_S(up);
407
408     /* Initialize uu on all grid points. */
409     mm1 = mm - 1;
410     for (j = 0; j < mm; j++) {
411         yfact = data->dx * j;

```

```

412     offset = mm*j;
413     for (i = 0; i < mm; i++) {
414         xfact = data->dx * i;
415         loc = offset + i;
416         udata[loc] = RCONST(16.0) * xfact * (ONE - xfact) * yfact * (ONE - yfact);
417     }
418 }
419
420 /* Initialize up vector to 0. */
421 N_VConst(ZERO, up);
422
423 /* resHeat sets res to negative of ODE RHS values at interior points. */
424 resHeat(ZERO, uu, up, res, data);
425
426 /* Copy -res into up to get correct interior initial up values. */
427 N_VScale(-ONE, res, up);
428
429 /* Set up at boundary points to zero. */
430 for (j = 0; j < mm; j++) {
431     offset = mm*j;
432     for (i = 0; i < mm; i++) {
433         loc = offset + i;
434         if (j == 0 || j == mm1 || i == 0 || i == mm1) updata[loc] = ZERO;
435     }
436 }
437
438 return(0);
439 }
440
441 /*
442 * Print first lines of output (problem description)
443 */
444
445 static void PrintHeader(realtype rtol, realtype atol)
446 {
447     printf("\nidakryx: Heat equation, serial example problem for IDA\n");
448     printf("Discretized heat equation on 2D unit square.\n");
449     printf("Zero boundary conditions,");
450     printf("initial conditions.\n");
451     printf("Mesh dimensions: %d x %d", MGRID, MGRID);
452     printf("Total system size: %d\n", NEQ);
453 #if defined(SUNDIALS_EXTENDED_PRECISION)
454     printf("Tolerance parameters: rtol=%Lg, atol=%Lg\n", rtol, atol);
455 #elif defined(SUNDIALS_DOUBLE_PRECISION)
456     printf("Tolerance parameters: rtol=%lg, atol=%lg\n", rtol, atol);
457 #else
458     printf("Tolerance parameters: rtol=%g, atol=%g\n", rtol, atol);
459 #endif
460     printf("Constraints set to force all solution components >= 0.\n");
461     printf("Linear solver: IDASPGMR, preconditioner using diagonal elements.\n");
462 }
463
464 /*
465 * PrintOutput: print max norm of solution and current solver statistics
466 */
467
468 static void PrintOutput(void *mem, realtype t, N_Vector uu)
469 {
470     realtype hused, umax;

```

```

471 long int nst, nni, nje, nre, nreLS, nli, npe, nps;
472 int kused, ier;
473
474 umax = N_VMaxNorm(uu);
475
476 ier = IDAGetLastOrder(mem, &kused);
477 check_flag(&ier, "IDAGetLastOrder", 1);
478 ier = IDAGetNumSteps(mem, &nst);
479 check_flag(&ier, "IDAGetNumSteps", 1);
480 ier = IDAGetNumNonlinSolvIter(mem, &nni);
481 check_flag(&ier, "IDAGetNumNonlinSolvIter", 1);
482 ier = IDAGetNumResEvals(mem, &nre);
483 check_flag(&ier, "IDAGetNumResEvals", 1);
484 ier = IDAGetLastStep(mem, &hused);
485 check_flag(&ier, "IDAGetLastStep", 1);
486 ier = IDASpilsGetNumJtimesEvals(mem, &nje);
487 check_flag(&ier, "IDASpilsGetNumJtimesEvals", 1);
488 ier = IDASpilsGetNumLinIter(mem, &nli);
489 check_flag(&ier, "IDASpilsGetNumLinIter", 1);
490 ier = IDASpilsGetNumResEvals(mem, &nreLS);
491 check_flag(&ier, "IDASpilsGetNumResEvals", 1);
492 ier = IDASpilsGetNumPrecEvals(mem, &npe);
493 check_flag(&ier, "IDASpilsGetPrecEvals", 1);
494 ier = IDASpilsGetNumPrecSolves(mem, &nps);
495 check_flag(&ier, "IDASpilsGetNumPrecSolves", 1);
496
497 #if defined(SUNDIALS_EXTENDED_PRECISION)
498 printf(" %5.2Lf %13.5Le %d %3ld %3ld %3ld %4ld %4ld %9.2Le %3ld %3ld\n",
499     t, umax, kused, nst, nni, nje, nre, nreLS, hused, npe, nps);
500 #elif defined(SUNDIALS_DOUBLE_PRECISION)
501 printf(" %5.2f %13.5e %d %3ld %3ld %3ld %4ld %4ld %9.2le %3ld %3ld\n",
502     t, umax, kused, nst, nni, nje, nre, nreLS, hused, npe, nps);
503 #else
504     printf(" %5.2f %13.5e %d %3ld %3ld %3ld %4ld %4ld %9.2e %3ld %3ld\n",
505         t, umax, kused, nst, nni, nje, nre, nreLS, hused, npe, nps);
506 #endif
507 }
508
509 /*
510 * Check function return value...
511 *   opt == 0 means SUNDIALS function allocates memory so check if
512 *           returned NULL pointer
513 *   opt == 1 means SUNDIALS function returns a flag so check if
514 *           flag >= 0
515 *   opt == 2 means function allocates memory so check if returned
516 *           NULL pointer
517 */
518
519 static int check_flag(void *flagvalue, char *funcname, int opt)
520 {
521     int *errflag;
522
523     /* Check if SUNDIALS function returned NULL pointer - no memory allocated */
524     if (opt == 0 && flagvalue == NULL) {
525         fprintf(stderr,
526                 "\nSUNDIALS_ERROR: %s() failed - returned NULL pointer\n\n",
527                 funcname);
528         return(1);
529     } else if (opt == 1) {

```

```
530     /* Check if flag < 0 */
531     errflag = (int *) flagvalue;
532     if (*errflag < 0) {
533         fprintf(stderr,
534                 "\nSUNDIALS_ERROR:\u%s() failed\u with\u flag\u=%d\n\n",
535                 funcname, *errflag);
536         return(1);
537     }
538 } else if (opt == 2 && flagvalue == NULL) {
539     /* Check if function returned NULL pointer - no memory allocated */
540     fprintf(stderr,
541             "\nMEMORY_ERROR:\u%s() failed\u -\u returned\u NULL\u pointer\n\n",
542             funcname);
543     return(1);
544 }
545
546     return(0);
547 }
```

D Listing of idakryx1.p.c

```

1  /*
2  * -----
3  * $Revision: 1.6 $
4  * $Date: 2006/03/17 16:58:01 $
5  * -----
6  * Programmer(s): Allan Taylor, Alan Hindmarsh and
7  *                 Radu Serban @ LLNL
8  * -----
9  * Example problem for IDA: 2D heat equation, parallel, GMRES.
10 *
11 * This example solves a discretized 2D heat equation problem.
12 * This version uses the Krylov solver IDASpgmr.
13 *
14 * The DAE system solved is a spatial discretization of the PDE
15 *      du/dt = d^2u/dx^2 + d^2u/dy^2
16 * on the unit square. The boundary condition is u = 0 on all edges.
17 * Initial conditions are given by u = 16 x (1 - x) y (1 - y).
18 * The PDE is treated with central differences on a uniform MX x MY
19 * grid. The values of u at the interior points satisfy ODEs, and
20 * equations u = 0 at the boundaries are appended, to form a DAE
21 * system of size N = MX * MY. Here MX = MY = 10.
22 *
23 * The system is actually implemented on submeshes, processor by
24 * processor, with an MXSUB by MYSUB mesh on each of NPEX * NPEY
25 * processors.
26 *
27 * The system is solved with IDA using the Krylov linear solver
28 * IDASPGMR. The preconditioner uses the diagonal elements of the
29 * Jacobian only. Routines for preconditioning, required by
30 * IDASPGMR, are supplied here. The constraints u >= 0 are posed
31 * for all components. Local error testing on the boundary values
32 * is suppressed. Output is taken at t = 0, .01, .02, .04,
33 * ..., 10.24.
34 * -----
35 */
36
37 #include <stdio.h>
38 #include <stdlib.h>
39 #include <math.h>
40
41 #include "ida.h"           /* Main header file */
42 #include "nvector_parallel.h" /* Definitions of N_Vector and NV_DATA_P */
43 #include "ida_spgrmr.h"     /* Use IDASPGMR linear solver */
44 #include "sundials_types.h" /* Definitions of realtype and booleantype */
45 #include "sundials_math.h"  /* Contains RSqrt routine */
46
47 #include "mpi.h"           /* MPI library routines */
48
49 #define ZERO  RCONST(0.0)
50 #define ONE   RCONST(1.0)
51 #define TWO   RCONST(2.0)
52
53 #define NOUT       11          /* Number of output times */
54
55 #define NPEX       2           /* No. PEs in x direction of PE array */
56 #define NPEY       2           /* No. PEs in y direction of PE array */
57                                         /* Total no. PEs = NPEX*NPEY */

```

```

58 #define MXSUB      5          /* No. x points per subgrid */
59 #define MYSUB      5          /* No. y points per subgrid */
60
61 #define MX          (NPEX*MXSUB)    /* MX = number of x mesh points */
62 #define MY          (NPEY*MYSUB)    /* MY = number of y mesh points */
63                                     /* Spatial mesh is MX by MY */
64
65 typedef struct {
66     long int thispe, mx, my, ixsub, jysub, npex, npey, mxsub, mysub;
67     realtype dx, dy, coeffx, coeffy, coeffxy;
68     realtype uext[(MXSUB+2)*(MYSUB+2)];
69     N_Vector pp;    /* vector of diagonal preconditioner elements */
70     MPI_Comm comm;
71 } *UserData;
72
73 /* User-supplied residual function and supporting routines */
74
75 int resHeat(realtype tt,
76             N_Vector uu, N_Vector up, N_Vector rr,
77             void *res_data);
78
79 static int rescomm(N_Vector uu, N_Vector up, void *res_data);
80
81 static int reslocal(realtype tt, N_Vector uu, N_Vector up,
82                      N_Vector res, void *res_data);
83
84 static int BSend(MPI_Comm comm, long int thispe, long int ixsub, long int jysub,
85                  long int dsizex, long int dsizey, realtype uarray[]);
86
87 static int BRecvPost(MPI_Comm comm, MPI_Request request[], long int thispe,
88                      long int ixsub, long int jysub,
89                      long int dsizex, long int dsizey,
90                      realtype uext[], realtype buffer[]);
91
92 static int BRecvWait(MPI_Request request[], long int ixsub, long int jysub,
93                      long int dsizex, realtype uext[], realtype buffer[]);
94
95 /* User-supplied preconditioner routines */
96
97 int PsolveHeat(realtype tt,
98                 N_Vector uu, N_Vector up, N_Vector rr,
99                 N_Vector rvec, N_Vector zvec,
100                realtype c_j, realtype delta, void *prec_data,
101                N_Vector tmp);
102
103 int PsetupHeat(realtype tt,
104                 N_Vector yy, N_Vector yp, N_Vector rr,
105                 realtype c_j, void *prec_data,
106                 N_Vector tmp1, N_Vector tmp2, N_Vector tmp3);
107
108 /* Private function to check function return values */
109
110 static int InitUserData(int thispe, MPI_Comm comm, UserData data);
111
112 static int SetInitialProfile(N_Vector uu, N_Vector up, N_Vector id,
113                             N_Vector res, UserData data);
114
115 static void PrintHeader(long int Neq, realtype rtol, realtype atol);
116

```

```

117 static void PrintOutput(int id, void *mem, realtype t, N_Vector uu);
118
119 static void PrintFinalStats(void *mem);
120
121 static int check_flag(void *flagvalue, char *funcname, int opt, int id);
122
123 /*
124 *-----*
125 * MAIN PROGRAM
126 *-----*
127 */
128
129 int main(int argc, char *argv[])
130 {
131     MPI_Comm comm;
132     void *mem;
133     UserData data;
134     int iout, thispe, ier, npes;
135     long int Neq, local_N;
136     realtype rtol, atol, t0, t1, tout, tret;
137     N_Vector uu, up, constraints, id, res;
138
139     mem = NULL;
140     data = NULL;
141     uu = up = constraints = id = res = NULL;
142
143     /* Get processor number and total number of pe's. */
144
145     MPI_Init(&argc, &argv);
146     comm = MPI_COMM_WORLD;
147     MPI_Comm_size(comm, &npes);
148     MPI_Comm_rank(comm, &thispe);
149
150     if (npes != NPEX*NPEY) {
151         if (thispe == 0)
152             fprintf(stderr,
153                     "\nMPI_ERROR(0): npes=%d is not equal to NPEX*NPEY=%d\n",
154                     npes, NPEX*NPEY);
155         MPI_Finalize();
156         return(1);
157     }
158
159     /* Set local length local_N and global length Neq. */
160
161     local_N = MXSUB*MYSUB;
162     Neq      = MX * MY;
163
164     /* Allocate and initialize the data structure and N-vectors. */
165
166     data = (UserData) malloc(sizeof *data);
167     data->pp = NULL;
168     if(check_flag((void *)data, "malloc", 2, thispe))
169         MPI_Abort(comm, 1);
170
171     uu = N_VNew_Parallel(comm, local_N, Neq);
172     if(check_flag((void *)uu, "N_VNew_Parallel", 0, thispe))
173         MPI_Abort(comm, 1);
174
175     up = N_VNew_Parallel(comm, local_N, Neq);

```

```

176 if(check_flag((void *)up, "N_VNew_Parallel", 0, thispe))
177     MPI_Abort(comm, 1);
178
179 res = N_VNew_Parallel(comm, local_N, Neq);
180 if(check_flag((void *)res, "N_VNew_Parallel", 0, thispe))
181     MPI_Abort(comm, 1);
182
183 constraints = N_VNew_Parallel(comm, local_N, Neq);
184 if(check_flag((void *)constraints, "N_VNew_Parallel", 0, thispe))
185     MPI_Abort(comm, 1);
186
187 id = N_VNew_Parallel(comm, local_N, Neq);
188 if(check_flag((void *)id, "N_VNew_Parallel", 0, thispe))
189     MPI_Abort(comm, 1);
190
191 /* An N-vector to hold preconditioner. */
192 data->pp = N_VNew_Parallel(comm, local_N, Neq);
193 if(check_flag((void *)data->pp, "N_VNew_Parallel", 0, thispe))
194     MPI_Abort(comm, 1);
195
196 InitUserData(thispe, comm, data);
197
198 /* Initialize the uu, up, id, and res profiles. */
199
200 SetInitialProfile(uu, up, id, res, data);
201
202 /* Set constraints to all 1's for nonnegative solution values. */
203
204 N_VConst(ONE, constraints);
205
206 t0 = ZERO; t1 = RCONST(0.01);
207
208 /* Scalar relative and absolute tolerance. */
209
210 rtol = ZERO;
211 atol = RCONST(1.0e-3);
212
213 /* Call IDACreate and IDAMalloc to initialize solution. */
214
215 mem = IDACreate();
216 if(check_flag((void *)mem, "IDACreate", 0, thispe)) MPI_Abort(comm, 1);
217
218 ier = IDASetRdata(mem, data);
219 if(check_flag(&ier, "IDASetRdata", 1, thispe)) MPI_Abort(comm, 1);
220
221 ier = IDASetSuppressAlg(mem, TRUE);
222 if(check_flag(&ier, "IDASetSuppressAlg", 1, thispe)) MPI_Abort(comm, 1);
223
224 ier = IDASetId(mem, id);
225 if(check_flag(&ier, "IDASetId", 1, thispe)) MPI_Abort(comm, 1);
226
227 ier = IDASetConstraints(mem, constraints);
228 if(check_flag(&ier, "IDASetConstraints", 1, thispe)) MPI_Abort(comm, 1);
229 N_VDestroy_Parallel(constraints);
230
231 ier = IDAMalloc(mem, resHeat, t0, uu, up, IDA_SS, rtol, &atol);
232 if(check_flag(&ier, "IDAMalloc", 1, thispe)) MPI_Abort(comm, 1);
233
234 /* Call IDASpgmr to specify the linear solver. */

```

```

235     ier = IDASpgmr(mem, 0);
236     if(check_flag(&ier, "IDASpgmr", 1, thispe)) MPI_Abort(comm, 1);
237
238     ier = IDASpilsSetPreconditioner(mem, PsetupHeat, PsolveHeat, data);
239     if(check_flag(&ier, "IDASpilsSetPreconditioner", 1, thispe)) MPI_Abort(comm, 1);
240
241     /* Print output heading (on processor 0 only) and intial solution */
242
243     if (thispe == 0) PrintHeader(Neq, rtol, atol);
244     PrintOutput(thispe, mem, t0, uu);
245
246     /* Loop over tout, call IDASolve, print output. */
247
248     for (tout = t1, iout = 1; iout <= NOUT; iout++, tout *= TWO) {
249
250         ier = IDASolve(mem, tout, &tret, uu, up, IDA_NORMAL);
251         if(check_flag(&ier, "IDASolve", 1, thispe)) MPI_Abort(comm, 1);
252
253         PrintOutput(thispe, mem, tret, uu);
254
255     }
256
257     /* Print remaining counters. */
258
259     if (thispe == 0) PrintFinalStats(mem);
260
261     /* Free memory */
262
263     IDAFree(&mem);
264
265     N_VDestroy_Parallel(id);
266     N_VDestroy_Parallel(res);
267     N_VDestroy_Parallel(up);
268     N_VDestroy_Parallel(uu);
269
270     N_VDestroy_Parallel(data->pp);
271     free(data);
272
273     MPI_Finalize();
274
275     return(0);
276
277 }
278
279 /*
280 *-----*
281 * FUNCTIONS CALLED BY IDA
282 *-----*
283 */
284
285 /*
286 * resHeat: heat equation system residual function
287 * This uses 5-point central differencing on the interior points, and
288 * includes algebraic equations for the boundary values.
289 * So for each interior point, the residual component has the form
290 *   res_i = u'_i - (central difference)_i
291 * while for each boundary point, it is res_i = u_i.
292 *
293 */

```

```

294 * This parallel implementation uses several supporting routines.
295 * First a call is made to rescomm to do communication of subgrid boundary
296 * data into array uext. Then reslocal is called to compute the residual
297 * on individual processors and their corresponding domains. The routines
298 * BSend, BRecvPost, and BRecvWait handle interprocessor communication
299 * of uu required to calculate the residual.
300 */
301
302 int resHeat(realtype tt,
303             N_Vecor uu, N_Vecor up, N_Vecor rr,
304             void *res_data)
305 {
306     int retval;
307
308     /* Call rescomm to do inter-processor communication. */
309     retval = rescomm(uu, up, res_data);
310
311     /* Call reslocal to calculate res. */
312     retval = reslocal(tt, uu, up, rr, res_data);
313
314     return(0);
315 }
316
317 /*
318 * PsetupHeat: setup for diagonal preconditioner for heatsk.
319 *
320 * The optional user-supplied functions PsetupHeat and
321 * PsolveHeat together must define the left preconditioner
322 * matrix P approximating the system Jacobian matrix
323 *  $J = dF/du + cj * dF/du'$ 
324 * (where the DAE system is  $F(t, u, u') = 0$ ), and solve the linear
325 * systems  $P z = r$ . This is done in this case by keeping only
326 * the diagonal elements of the J matrix above, storing them as
327 * inverses in a vector pp, when computed in PsetupHeat, for
328 * subsequent use in PsolveHeat.
329 *
330 * In this instance, only cj and data (user data structure, with
331 * pp etc.) are used from the PsetupHeat argument list.
332 *
333 */
334
335
336 int PsetupHeat(realtype tt,
337                 N_Vecor yy, N_Vecor yp, N_Vecor rr,
338                 realtype c_j, void *prec_data,
339                 N_Vecor tmp1, N_Vecor tmp2, N_Vecor tmp3)
340 {
341     realtype *ppv, pelinv;
342     long int lx, ly, ixbegin, ixend, jybegin, jyend, locu, mxsub, mysub;
343     long int ixsub, jysub, npex, npey;
344     UserData data;
345
346     data = (UserData) prec_data;
347
348     ppv = NV_DATA_P(data->pp);
349     ixsub = data->ixsub;
350     jysub = data->jysub;
351     mxsub = data->mxsub;
352     mysub = data->mysub;

```

```

353     npex  = data->npex;
354     npey  = data->npey;
355
356     /* Initially set all pp elements to one. */
357     N_VConst(ONE, data->pp);
358
359     /* Prepare to loop over subgrid. */
360     ixbegin = 0;
361     ixend   = mxsub-1;
362     jybegin = 0;
363     jyend   = mysub-1;
364     if (ixsub == 0) ixbegin++; if (ixsub == npex-1) ixend--;
365     if (jysub == 0) jybegin++; if (jysub == npey-1) jyend--;
366     pelinv = ONE/(c_j + data->coeffxy);
367
368     /* Load the inverse of the preconditioner diagonal elements
369      in loop over all the local subgrid. */
370
371     for (ly = jybegin; ly <=jyend; ly++) {
372         for (lx = ixbegin; lx <= ixend; lx++) {
373             locu = lx + ly*mxsub;
374             ppv[locu] = pelinv;
375         }
376     }
377
378     return(0);
379
380 }
381
382 /*
383 * PsolveHeat: solve preconditioner linear system.
384 * This routine multiplies the input vector rvec by the vector pp
385 * containing the inverse diagonal Jacobian elements (previously
386 * computed in PsetupHeat), returning the result in zvec.
387 */
388
389 int PsolveHeat(realtype tt,
390                 N_Vector uu, N_Vector up, N_Vector rr,
391                 N_Vector rvec, N_Vector zvec,
392                 realtype c_j, realtype delta, void *prec_data,
393                 N_Vector tmp)
394 {
395     UserData data;
396
397     data = (UserData) prec_data;
398
399     N_VProd(data->pp, rvec, zvec);
400
401     return(0);
402
403 }
404
405 /*
406 *-----*
407 * SUPPORTING FUNCTIONS
408 *-----*
409 */
410
411

```

```

412 /*
413  * rescomm routine. This routine performs all inter-processor
414  * communication of data in uu needed to calculate G.
415 */
416
417 static int rescomm(N_Vecor uu, N_Vecor up, void *res_data)
418 {
419     UserData data;
420     realtype *uarray, *uext, buffer[2*MYSUB];
421     MPI_Comm comm;
422     long int thispe, ixsub, jysub, mxsub, mysub;
423     MPI_Request request[4];
424
425     data = (UserData) res_data;
426     uarray = NV_DATA_P(uu);
427
428     /* Get comm, thispe, subgrid indices, data sizes, extended array uext. */
429     comm = data->comm; thispe = data->thispe;
430     ixsub = data->ixsub; jysub = data->jysub;
431     mxsub = data->mxsub; mysub = data->mysub;
432     uext = data->uext;
433
434     /* Start receiving boundary data from neighboring PEs. */
435     BRecvPost(comm, request, thispe, ixsub, jysub, mxsub, mysub, uext, buffer);
436
437     /* Send data from boundary of local grid to neighboring PEs. */
438     BSend(comm, thispe, ixsub, jysub, mxsub, mysub, uarray);
439
440     /* Finish receiving boundary data from neighboring PEs. */
441     BRecvWait(request, ixsub, jysub, mxsub, uext, buffer);
442
443     return(0);
444
445 }
446
447 /*
448  * reslocal routine. Compute res = F(t, uu, up). This routine assumes
449  * that all inter-processor communication of data needed to calculate F
450  * has already been done, and that this data is in the work array uext.
451 */
452
453 static int reslocal(realtype tt,
454                      N_Vecor uu, N_Vecor up, N_Vecor rr,
455                      void *res_data)
456 {
457     realtype *uext, *uuv, *upv, *resv;
458     realtype termx, termy, termctr;
459     long int lx, ly, offsetu, offsetue, locu, locue;
460     long int ixsub, jysub, mxsub, mxsub2, mysub, npex, npey;
461     long int ixbegin, ixend, jybegin, jyend;
462     UserData data;
463
464     /* Get subgrid indices, array sizes, extended work array uext. */
465
466     data = (UserData) res_data;
467     uext = data->uext;
468     uuv = NV_DATA_P(uu);
469     upv = NV_DATA_P(up);
470     resv = NV_DATA_P(rr);

```

```

471 ixsub = data->ixsub; jysub = data->jysub;
472 mxsub = data->mxsub; mxsub2 = data->mxsub + 2;
473 mysub = data->mysub; npex = data->npex; npey = data->npey;
474
475 /* Initialize all elements of rr to uu. This sets the boundary
476    elements simply without indexing hassles. */
477
478 N_VScale(ONE, uu, rr);
479
480 /* Copy local segment of u vector into the working extended array uext.
481    This completes uext prior to the computation of the rr vector.      */
482
483 offsetu = 0;
484 offsetue = mxsub2 + 1;
485 for (ly = 0; ly < mysub; ly++) {
486     for (lx = 0; lx < mxsub; lx++) uext[offsetue+lx] = uuv[offsetu+lx];
487     offsetu = offsetu + mxsub;
488     offsetue = offsetue + mxsub2;
489 }
490
491 /* Set loop limits for the interior of the local subgrid. */
492
493 ixbegin = 0;
494 ixend = mxsub-1;
495 jybegin = 0;
496 jyend = mysub-1;
497 if (ixsub == 0) ixbegin++; if (ixsub == npex-1) ixend--;
498 if (jysub == 0) jybegin++; if (jysub == npey-1) jyend--;
499
500 /* Loop over all grid points in local subgrid. */
501
502 for (ly = jybegin; ly <= jyend; ly++) {
503     for (lx = ixbegin; lx <= ixend; lx++) {
504         locu = lx + ly*mxsub;
505         locue = (lx+1) + (ly+1)*mxsub2;
506         termx = data->coeffx *(uext[locue-1]      + uext[locue+1]);
507         termy = data->coeffy *(uext[locue-mxsub2] + uext[locue+mxsub2]);
508         termctr = data->coeffxy*uext[locue];
509         resv[locu] = upv[locu] - (termx + termy - termctr);
510     }
511 }
512 return(0);
513
514 }
515
516 /*
517 * Routine to send boundary data to neighboring PEs.
518 */
519
520 static int BSend(MPI_Comm comm, long int thispe, long int ixsub, long int jysub,
521                  long int dsizex, long int dsizey, realtype uarray[])
522 {
523     long int ly, offsetu;
524     realtype bufleft[MYSUB], bufright[MYSUB];
525
526     /* If jysub > 0, send data from bottom x-line of u. */
527
528     if (jysub != 0)
529         MPI_Send(&uarray[0], dsizex, PVEC_REAL_MPI_TYPE, thispe-NPEX, 0, comm);

```

```

530
531     /* If jysub < NPEY-1, send data from top x-line of u. */
532
533     if (jysub != NPEY-1) {
534         offsetu = (MYSUB-1)*dsizex;
535         MPI_Send(&uarray[offsetu], dsizex, PVEC_REAL_MPI_TYPE,
536                  thispe+NPEX, 0, comm);
537     }
538
539     /* If ixsub > 0, send data from left y-line of u (via bufleft). */
540
541     if (ixsub != 0) {
542         for (ly = 0; ly < MYSUB; ly++) {
543             offsetu = ly*dsizex;
544             bufleft[ly] = uarray[offsetu];
545         }
546         MPI_Send(&bufleft[0], dsizey, PVEC_REAL_MPI_TYPE, thispe-1, 0, comm);
547     }
548
549     /* If ixsub < NPEX-1, send data from right y-line of u (via bufright). */
550
551     if (ixsub != NPEX-1) {
552         for (ly = 0; ly < MYSUB; ly++) {
553             offsetu = ly*MXSUB + (MXSUB-1);
554             bufright[ly] = uarray[offsetu];
555         }
556         MPI_Send(&bufright[0], dsizey, PVEC_REAL_MPI_TYPE, thispe+1, 0, comm);
557     }
558
559     return(0);
560 }
561
562 /*
563 * Routine to start receiving boundary data from neighboring PEs.
564 * Notes:
565 *   1) buffer should be able to hold 2*MYSUB realtype entries, should be
566 *      passed to both the BRecvPost and BRecvWait functions, and should not
567 *      be manipulated between the two calls.
568 *   2) request should have 4 entries, and should be passed in
569 *      both calls also.
570 */
571
572 static int BRecvPost(MPI_Comm comm, MPI_Request request[], long int thispe,
573                      long int ixsub, long int jysub,
574                      long int dsizex, long int dsizey,
575                      realtype uext[], realtype buffer[])
576 {
577     long int offsetue;
578     /* Have bufleft and bufright use the same buffer. */
579     realtype *bufleft = buffer, *bufright = buffer+MYSUB;
580
581     /* If jysub > 0, receive data for bottom x-line of uext. */
582     if (jysub != 0)
583         MPI_Irecv(&uext[1], dsizex, PVEC_REAL_MPI_TYPE,
584                   thispe-NPEX, 0, comm, &request[0]);
585
586     /* If jysub < NPEY-1, receive data for top x-line of uext. */
587     if (jysub != NPEY-1) {

```

```

589     offsetue = (1 + (MYSUB+1)*(MXSUB+2));
590     MPI_Irecv(&uext[offsetue], dsizex, PVEC_REAL_MPI_TYPE,
591                 thispe+NPEX, 0, comm, &request[1]);
592 }
593
594 /* If ixsub > 0, receive data for left y-line of uext (via bufleft). */
595 if (ixsub != 0) {
596     MPI_Irecv(&bufleft[0], dsizey, PVEC_REAL_MPI_TYPE,
597                 thispe-1, 0, comm, &request[2]);
598 }
599
600 /* If ixsub < NPEX-1, receive data for right y-line of uext (via bufright). */
601 if (ixsub != NPEX-1) {
602     MPI_Irecv(&bufright[0], dsizey, PVEC_REAL_MPI_TYPE,
603                 thispe+1, 0, comm, &request[3]);
604 }
605
606 return(0);
607
608 }
609
610 /*
611 * Routine to finish receiving boundary data from neighboring PEs.
612 * Notes:
613 *   1) buffer should be able to hold 2*MYSUB realtype entries, should be
614 *      passed to both the BRecvPost and BRecvWait functions, and should not
615 *      be manipulated between the two calls.
616 *   2) request should have four entries, and should be passed in both
617 *      calls also.
618 */
619
620 static int BRecvWait(MPI_Request request[], long int ixsub, long int jysub,
621                      long int dsizex, realtype uext[], realtype buffer[])
622 {
623     long int ly, dsizex2, offsetue;
624     realtype *bufleft = buffer, *bufright = buffer+MYSUB;
625     MPI_Status status;
626
627     dsizex2 = dsizex + 2;
628
629     /* If jysub > 0, receive data for bottom x-line of uext. */
630     if (jysub != 0)
631         MPI_Wait(&request[0],&status);
632
633     /* If jysub < NPEY-1, receive data for top x-line of uext. */
634     if (jysub != NPEY-1)
635         MPI_Wait(&request[1],&status);
636
637     /* If ixsub > 0, receive data for left y-line of uext (via bufleft). */
638     if (ixsub != 0) {
639         MPI_Wait(&request[2],&status);
640
641         /* Copy the buffer to uext. */
642         for (ly = 0; ly < MYSUB; ly++) {
643             offsetue = (ly+1)*dsizex2;
644             uext[offsetue] = bufleft[ly];
645         }
646     }
647 }

```

```

648 /* If ixsub < NPEX-1, receive data for right y-line of uext (via bufright). */
649 if (ixsub != NPEX-1) {
650     MPI_Wait(&request[3],&status);
651
652     /* Copy the buffer to uext */
653     for (ly = 0; ly < MYSUB; ly++) {
654         offsetue = (ly+2)*dsizex2 - 1;
655         uext[offsetue] = bufright[ly];
656     }
657 }
658
659 return(0);
660
661 }
662
663 /*
664 *-----*
665 * PRIVATE FUNCTIONS
666 *-----*
667 */
668
669 /*
670 * InitUserData initializes the user's data block data.
671 */
672
673 static int InitUserData(int thispe, MPI_Comm comm, UserData data)
674 {
675     data->thispe = thispe;
676     data->dx = ONE/(MX-ONE);           /* Assumes a [0,1] interval in x. */
677     data->dy = ONE/(MY-ONE);           /* Assumes a [0,1] interval in y. */
678     data->coeffx = ONE/(data->dx * data->dx);
679     data->coeffy = ONE/(data->dy * data->dy);
680     data->coeffxy = TWO/(data->dx * data->dx) + TWO/(data->dy * data->dy) ;
681     data->jysub = thispe/NPEX;
682     data->ixsub = thispe - data->jysub * NPEX;
683     data->npxe = NPEX;
684     data->npey = NPEY;
685     data->mx = MX;
686     data->my = MY;
687     data->mxsub = MXSUB;
688     data->mysub = MYSUB;
689     data->comm = comm;
690     return(0);
691
692 }
693
694 /*
695 * SetInitialProfile sets the initial values for the problem.
696 */
697
698 static int SetInitialProfile(N_Vector uu, N_Vector up, N_Vector id,
699                             N_Vector res, UserData data)
700 {
701     long int i, iloc, j, jloc, offset, loc, ixsub, jysub;
702     long int ixbegin, ixend, jybegin, jyend;
703     realtype xfact, yfact, *udata, *iddata, dx, dy;
704
705     /* Initialize uu. */
706

```

```

707     udata = NV_DATA_P(uu);
708     iddata = NV_DATA_P(id);
709
710     /* Set mesh spacings and subgrid indices for this PE. */
711     dx = data->dx;
712     dy = data->dy;
713     ixsub = data->ixsub;
714     jysub = data->jysub;
715
716     /* Set beginning and ending locations in the global array corresponding
717      to the portion of that array assigned to this processor. */
718     ixbegin = MXSUB*ixsub;
719     ixend = MXSUB*(ixsub+1) - 1;
720     jybegin = MYSUB*jysub;
721     jyend = MYSUB*(jysub+1) - 1;
722
723     /* Loop over the local array, computing the initial profile value.
724      The global indices are (i,j) and the local indices are (iloc,jloc).
725      Also set the id vector to zero for boundary points, one otherwise. */
726
727     N_VConst(ONE,id);
728     for (j = jybegin, jloc = 0; j <= jyend; j++, jloc++) {
729         yfact = data->dy*j;
730         offset= jloc*MXSUB;
731         for (i = ixbegin, iloc = 0; i <= ixend; i++, iloc++) {
732             xfact = data->dx * i;
733             loc = offset + iloc;
734             udata[loc] = RCONST(16.0) * xfact * (ONE - xfact) * yfact * (ONE - yfact);
735             if (i == 0 || i == MX-1 || j == 0 || j == MY-1) iddata[loc] = ZERO;
736         }
737     }
738
739     /* Initialize up. */
740
741     N_VConst(ZERO, up);      /* Initially set up = 0. */
742
743     /* resHeat sets res to negative of ODE RHS values at interior points. */
744     resHeat(ZERO, uu, up, res, data);
745
746     /* Copy -res into up to get correct initial up values. */
747     N_VScale(-ONE, res, up);
748
749     return(0);
750 }
751
752 /*
753  * Print first lines of output and table heading
754 */
755
756 static void PrintHeader(long int Neq, realtype rtol, realtype atol)
757 {
758     printf("\nidakryx1_p: Heat equation, parallel example problem for IDA\n");
759     printf("uuuuuuuuuuuu Discretized heat equation on 2D unit square.\n");
760     printf("uuuuuuuuuuuu Zero boundary conditions, ");
761     printf("upolynomial initial conditions.\n");
762     printf("uuuuuuuuuuuu Mesh dimensions: %d x %d", MX, MY);
763     printf("uuuuuuuuuu Total system size: %ld\n\n", Neq);
764     printf("Subgrid dimensions: %d x %d", MXSUB, MYSUB);
765     printf("uuuuuuuuuu Processor array: %d x %d\n", NPEX, NPEY);

```

```

766 #if defined(SUNDIALS_EXTENDED_PRECISION)
767   printf("Toleranceparameters:rtol=%Lguuuatol=%Lg\n", rtol, atol);
768 #elif defined(SUNDIALS_DOUBLE_PRECISION)
769   printf("Toleranceparameters:rtol=%lguuuatol=%lg\n", rtol, atol);
770 #else
771   printf("Toleranceparameters:rtol=%guuuatol=%g\n", rtol, atol);
772 #endif
773   printf("Constraintsset to force all solution components >= 0.\n");
774   printf("SUPPRESSALG = TRUE to suppress local error testing on ");
775   printf("all boundary components.\n");
776   printf("Linearsolver: IDASPGMR\n");
777   printf("Preconditioner: diagonal elements only.\n");
778
779 /* Print output table heading and initial line of table. */
780 printf("\nOutputSummary(umax = max norm of solution)\n\n");
781 printf(" time uuuuuuumax uuuuuuuuk uuuuuuuunst uuuuuuuunni uuuuuuuunre uuuuuuuunreLS uuuuuuuuh uuuuuuuunpe uuuuuuuunps\n");
782 printf("-----\n");
783 }
784
785 /*
786 * PrintOutput: print max norm of solution and current solver statistics
787 */
788
789 static void PrintOutput(int id, void *mem, realtype t, N_Vector uu)
790 {
791   realtype hused, umax;
792   long int nst, nni, nje, nre, nreLS, nli, npe, nps;
793   int kused, ier;
794
795   umax = N_VMaxNorm(uu);
796
797   if (id == 0) {
798
799     ier = IDAGetLastOrder(mem, &kused);
800     check_flag(&ier, "IDAGetLastOrder", 1, id);
801     ier = IDAGetNumSteps(mem, &nst);
802     check_flag(&ier, "IDAGetNumSteps", 1, id);
803     ier = IDAGetNumNonlinSolvIter(mem, &nni);
804     check_flag(&ier, "IDAGetNumNonlinSolvIter", 1, id);
805     ier = IDAGetNumResEvals(mem, &nre);
806     check_flag(&ier, "IDAGetNumResEvals", 1, id);
807     ier = IDAGetLastStep(mem, &hused);
808     check_flag(&ier, "IDAGetLastStep", 1, id);
809     ier = IDASpilsGetNumJtimesEvals(mem, &nje);
810     check_flag(&ier, "IDASpilsGetNumJtimesEvals", 1, id);
811     ier = IDASpilsGetNumLinIter(mem, &nli);
812     check_flag(&ier, "IDASpilsGetNumLinIter", 1, id);
813     ier = IDASpilsGetNumResEvals(mem, &nreLS);
814     check_flag(&ier, "IDASpilsGetNumResEvals", 1, id);
815     ier = IDASpilsGetNumPrecEvals(mem, &npe);
816     check_flag(&ier, "IDASpilsGetPrecEvals", 1, id);
817     ier = IDASpilsGetNumPrecSolves(mem, &nps);
818     check_flag(&ier, "IDASpilsGetNumPrecSolves", 1, id);
819
820 #if defined(SUNDIALS_EXTENDED_PRECISION)
821   printf(" %5.2Lf %13.5Le %d %3ld %3ld %3ld %4ld %4ld %9.2Le %3ld %3ld\n",
822         t, umax, kused, nst, nni, nje, nre, nreLS, hused, npe, nps);
823 #elif defined(SUNDIALS_DOUBLE_PRECISION)
824   printf(" %5.2f %13.5e %d %3ld %3ld %3ld %4ld %4ld %9.2le %3ld %3ld\n",

```

```

825             t, umax, kused, nst, nni, nje, nre, nreLS, hused, npe, nps);
826 #else
827     printf(" %5.2f %13.5e %d %3ld %3ld %3ld %4ld %4ld %9.2e %3ld %3ld\n",
828            t, umax, kused, nst, nni, nje, nre, nreLS, hused, npe, nps);
829 #endif
830     }
831 }
833
834 /*
835 * Print some final integrator statistics
836 */
837
838 static void PrintFinalStats(void *mem)
839 {
840     long int netf, ncfn, ncfl;
841
842     IDAGetNumErrTestFails(mem, &netf);
843     IDAGetNumNonlinSolvConvFails(mem, &ncfn);
844     IDASpilsGetNumConvFails(mem, &ncfl);
845
846     printf("\nError test failures = %ld\n", netf);
847     printf("Nonlinear convergence failures = %ld\n", ncfn);
848     printf("Linear convergence failures = %ld\n", ncfl);
849 }
850
851 /*
852 * Check function return value...
853 * opt == 0 means SUNDIALS function allocates memory so check if
854 *           returned NULL pointer
855 * opt == 1 means SUNDIALS function returns a flag so check if
856 *           flag >= 0
857 * opt == 2 means function allocates memory so check if returned
858 *           NULL pointer
859 */
860
861 static int check_flag(void *flagvalue, char *funcname, int opt, int id)
862 {
863     int *errflag;
864
865     if (opt == 0 && flagvalue == NULL) {
866         /* Check if SUNDIALS function returned NULL pointer - no memory allocated */
867         fprintf(stderr,
868                 "\nSUNDIALS_ERROR(%d): %s() failed - returned NULL pointer\n\n",
869                 id, funcname);
870         return(1);
871     } else if (opt == 1) {
872         /* Check if flag < 0 */
873         errflag = (int *) flagvalue;
874         if (*errflag < 0) {
875             fprintf(stderr,
876                     "\nSUNDIALS_ERROR(%d): %s() failed with flag = %d\n\n",
877                     id, funcname, *errflag);
878             return(1);
879         }
880     } else if (opt == 2 && flagvalue == NULL) {
881         /* Check if function returned NULL pointer - no memory allocated */
882         fprintf(stderr,
883                 "\nMEMORY_ERROR(%d): %s() failed - returned NULL pointer\n\n",

```

```
884         id, funcname);
885     return(1);
886 }
887
888 return(0);
889 }
```

E Listing of idakryx2_bbd_p.c

```

1  /*
2  * -----
3  * $Revision: 1.4 $
4  * $Date: 2006/03/17 16:58:01 $
5  * -----
6  * Programmer(s): Allan Taylor, Alan Hindmarsh and
7  *                 Radu Serban @ LLNL
8  * -----
9  * Example program for IDA: Food web, parallel, GMRES, IDABBD
10 * preconditioner.
11 *
12 * This example program for IDA uses IDASPGMR as the linear solver.
13 * It is written for a parallel computer system and uses the
14 * IDABBDPRE band-block-diagonal preconditioner module for the
15 * IDASPGMR package. It was originally run on a Sun SPARC cluster
16 * and used MPICH.
17 *
18 * The mathematical problem solved in this example is a DAE system
19 * that arises from a system of partial differential equations after
20 * spatial discretization. The PDE system is a food web population
21 * model, with predator-prey interaction and diffusion on the unit
22 * square in two dimensions. The dependent variable vector is:
23 *
24 *      1   2           ns
25 *  c = (c , c , ..., c ) , ns = 2 * np
26 *
27 * and the PDE's are as follows:
28 *
29 *      i           i           i
30 *  dc /dt = d(i)*(c    + c   ) + R (x,y,c)   (i = 1,...,np)
31 *                  xx       yy       i
32 *
33 *      i           i
34 *  0 = d(i)*(c    + c   ) + R (x,y,c)   (i = np+1,...,ns)
35 *                  xx       yy       i
36 *
37 * where the reaction terms R are:
38 *
39 *      i           ns           j
40 *  R (x,y,c) = c * (b(i) + sum a(i,j)*c )
41 *                  i                   j=1
42 *
43 * The number of species is ns = 2 * np, with the first np being
44 * prey and the last np being predators. The coefficients a(i,j),
45 * b(i), d(i) are:
46 *
47 *  a(i,i) = -AA (all i)
48 *  a(i,j) = -GG (i <= np , j > np)
49 *  a(i,j) = EE (i > np, j <= np)
50 *  all other a(i,j) = 0
51 *  b(i) = BB*(1+ alpha * x*y + beta*sin(4 pi x)*sin(4 pi y)) (i <= np)
52 *  b(i) = -BB*(1+ alpha * x*y + beta*sin(4 pi x)*sin(4 pi y)) (i > np)
53 *  d(i) = DPREY (i <= np)
54 *  d(i) = DPRED (i > np)
55 *
56 * Note: The above equations are written in 1-based indices,
57 * whereas the code has 0-based indices, being written in C.

```

```

58 *
59 * The various scalar parameters required are set using '#define'
60 * statements or directly in routine InitUserData. In this program,
61 * np = 1, ns = 2. The boundary conditions are homogeneous Neumann:
62 * normal derivative = 0.
63 *
64 * A polynomial in x and y is used to set the initial values of the
65 * first np variables (the prey variables) at each x,y location,
66 * while initial values for the remaining (predator) variables are
67 * set to a flat value, which is corrected by IDACalcIC.
68 *
69 * The PDEs are discretized by central differencing on a MX by MY
70 * mesh, and so the system size Neq is the product
71 * MX * MY * NUM_SPECIES. The system is actually implemented on
72 * submeshes, processor by processor, with an MXSUB by MYSUB mesh
73 * on each of NPEX * NPEY processors.
74 *
75 * The DAE system is solved by IDA using the IDASPGMR linear solver,
76 * in conjunction with the preconditioner module IDABBDPRE. The
77 * preconditioner uses a 5-diagonal band-block-diagonal
78 * approximation (half-bandwidths = 2). Output is printed at
79 * t = 0, .001, .01, .1, .4, .7, 1.
80 * -----
81 * References:
82 * [1] Peter N. Brown and Alan C. Hindmarsh,
83 *      Reduced Storage Matrix Methods in Stiff ODE systems,
84 *      Journal of Applied Mathematics and Computation, Vol. 31
85 *      (May 1989), pp. 40-91.
86 *
87 * [2] Peter N. Brown, Alan C. Hindmarsh, and Linda R. Petzold,
88 *      Using Krylov Methods in the Solution of Large-Scale
89 *      Differential-Algebraic Systems, SIAM J. Sci. Comput., 15
90 *      (1994), pp. 1467-1488.
91 *
92 * [3] Peter N. Brown, Alan C. Hindmarsh, and Linda R. Petzold,
93 *      Consistent Initial Condition Calculation for Differential-
94 *      Algebraic Systems, SIAM J. Sci. Comput., 19 (1998),
95 *      pp. 1495-1512.
96 * -----
97 */
98
99 #include <stdio.h>
100 #include <stdlib.h>
101 #include <math.h>
102
103 #include "ida.h"           /* Main header file */
104 #include "nvector_parallel.h" /* Definitions of N_Vector and NV_DATA_P */
105 #include "ida_spgmr.h"      /* Use IDASPGMR linear solver */
106 #include "ida_bbdpre.h"     /* Definitions for the IDABBDPRE prec. */
107 #include "sundials_smalldense.h" /* definition of denalloc */
108 #include "sundials_types.h"   /* Definitions of realtype and booleantype */
109 #include "sundials_math.h"    /* Contains RSqrt routine */
110
111 #include "mpi.h"           /* MPI library routines */
112
113 /* Problem Constants */
114
115 #define NPREY      1          /* Number of prey (= number of predators). */
116 #define NUM_SPECIES 2*NPREY

```

```

117
118 #define PI RCONST(3.1415926535898) /* pi */
119 #define FOURPI (RCONST(4.0)*PI) /* 4 pi */
120
121 #define MXSUB 10 /* Number of x mesh points per processor subgrid */
122 #define MYSUB 10 /* Number of y mesh points per processor subgrid */
123 #define NPEX 2 /* Number of subgrids in the x direction */
124 #define NPEY 2 /* Number of subgrids in the y direction */
125 #define MX (MXSUB*NPEX) /* MX = number of x mesh points */
126 #define MY (MYSUB*NPEY) /* MY = number of y mesh points */
127 #define NSMXSUB (NUM_SPECIES * MXSUB)
128 #define NEQ (NUM_SPECIES*MX*MY) /* Number of equations in system */
129 #define AA RCONST(1.0) /* Coefficient in above eqns. for a */
130 #define EE RCONST(10000.) /* Coefficient in above eqns. for a */
131 #define GG RCONST(0.5e-6) /* Coefficient in above eqns. for a */
132 #define BB RCONST(1.0) /* Coefficient in above eqns. for b */
133 #define DPREY RCONST(1.0) /* Coefficient in above eqns. for d */
134 #define DPRED RCONST(0.05) /* Coefficient in above eqns. for d */
135 #define ALPHA RCONST(50.) /* Coefficient alpha in above eqns. */
136 #define BETA RCONST(1000.) /* Coefficient beta in above eqns. */
137 #define AX RCONST(1.0) /* Total range of x variable */
138 #define AY RCONST(1.0) /* Total range of y variable */
139 #define RTOL RCONST(1.e-5) /* rtol tolerance */
140 #define ATOL RCONST(1.e-5) /* atol tolerance */
141 #define ZERO RCONST(0.) /* 0. */
142 #define ONE RCONST(1.0) /* 1. */
143 #define NOUT 6
144 #define TMULT RCONST(10.0) /* Multiplier for tout values */
145 #define TADD RCONST(0.3) /* Increment for tout values */
146
147 /* User-defined vector accessor macro IJ_Vptr. */
148 /*
149 *
150 * IJ_Vptr is defined in order to express the underlying 3-d structure of the
151 * dependent variable vector from its underlying 1-d storage (an N_Vector).
152 * IJ_Vptr(vv,i,j) returns a pointer to the location in vv corresponding to
153 * species index is = 0, x-index ix = i, and y-index jy = j.
154 */
155
156 #define IJ_Vptr(vv,i,j) (&NV_Ith_P(vv, (i)*NUM_SPECIES + (j)*NSMXSUB ))
157
158 /* Type: UserData. Contains problem constants, preconditioner data, etc. */
159
160 typedef struct {
161     long int ns, np, thispe, npes, ixsub, jysub, npex, npey;
162     long int mxsub, mysub, nsmxsub, nsmxsub2;
163     realtype dx, dy, **acoef;
164     realtype cox[NUM_SPECIES], coy[NUM_SPECIES], bcoef[NUM_SPECIES],
165             rhs[NUM_SPECIES], cext[(MXSUB+2)*(MYSUB+2)*NUM_SPECIES];
166     MPI_Comm comm;
167     N_Vector rates;
168     long int n_local;
169 } *UserData;
170
171 /* Prototypes for functions called by the IDA Solver. */
172
173 static int resweb(realtype tt,
174                   N_Vector cc, N_Vector cp, N_Vector rr,
175                   void *res_data);

```

```

176 static int reslocal(long int Nlocal, realtype tt,
177                     N_Vector cc, N_Vector cp, N_Vector res,
178                     void *res_data);
179
180 static int rescomm(long int Nlocal, realtype tt,
181                     N_Vector cc, N_Vector cp,
182                     void *res_data);
183
184 /* Prototypes for supporting functions */
185
186 static void BSend(MPI_Comm comm, long int thispe, long int ixsub, long int jysub,
187                     long int dsizex, long int dsizey, realtype carray[]);
188
189 static void BRecvPost(MPI_Comm comm, MPI_Request request[], long int thispe,
190                     long int ixsub, long int jysub,
191                     long int dsizex, long int dsizey,
192                     realtype cext[], realtype buffer[]);
193
194 static void BRecvWait(MPI_Request request[], long int ixsub, long int jysub,
195                     long int dsizex, realtype cext[], realtype buffer[]);
196
197 static void WebRates(realtype xx, realtype yy, realtype *cxy, realtype *ratesxy,
198                     UserData webdata);
199
200 static realtype dotprod(long int size, realtype *x1, realtype *x2);
201
202 /* Prototypes for private functions */
203
204 static void InitUserData(UserData webdata, int thispe, int npes,
205                         MPI_Comm comm);
206
207 static void SetInitialProfiles(N_Vector cc, N_Vector cp, N_Vector id,
208                               N_Vector scrtch, UserData webdata);
209
210 static void PrintHeader(long int SystemSize, int maxl,
211                         long int mudq, long int mldq,
212                         long int mukeep, long int mlkeep,
213                         realtype rtol, realtype atol);
214
215 static void PrintOutput(void *mem, N_Vector cc, realtype time,
216                         UserData webdata, MPI_Comm comm);
217
218 static void PrintFinalStats(void *mem, void *P_data);
219
220 static int check_flag(void *flagvalue, char *funcname, int opt, int id);
221
222 /*
223 *-----*
224 * MAIN PROGRAM
225 *-----*
226 */
227
228
229 int main(int argc, char *argv[])
230 {
231     MPI_Comm comm;
232     void *mem, *P_data;
233     UserData webdata;
234     long int SystemSize, local_N, mudq, mldq, mukeep, mlkeep;

```

```

235     realtype rtol, atol, t0, tout, tret;
236     N_Vector cc, cp, res, id;
237     int thispe, npes, maxl, iout, retval;
238
239     cc = cp = res = id = NULL;
240     webdata = NULL;
241     mem = P_data = NULL;
242
243     /* Set communicator, and get processor number and total number of PE's. */
244
245     MPI_Initialized(&argc, &argv);
246     comm = MPI_COMM_WORLD;
247     MPI_Comm_rank(comm, &thispe);
248     MPI_Comm_size(comm, &npes);
249
250     if (npes != NPEX*NPEY) {
251         if (thispe == 0)
252             fprintf(stderr,
253                     "\nMPI_ERROR(0): npes=%d not equal to NPEX*NPEY=%d\n",
254                     npes, NPEX*NPEY);
255         MPI_Finalize();
256         return(1);
257     }
258
259     /* Set local length (local_N) and global length (SystemSize). */
260
261     local_N = MXSUB*MYSUB*NUM_SPECIES;
262     SystemSize = NEQ;
263
264     /* Set up user data block webdata. */
265
266     webdata = (UserData) malloc(sizeof *webdata);
267     webdata->rates = N_VNew_Parallel(comm, local_N, SystemSize);
268     webdata->acoef = denalloc(NUM_SPECIES);
269
270     InitUserData(webdata, thispe, npes, comm);
271
272     /* Create needed vectors, and load initial values.
273        The vector res is used temporarily only. */
274
275     cc = N_VNew_Parallel(comm, local_N, SystemSize);
276     if(check_flag((void *)cc, "N_VNew_Parallel", 0, thispe)) MPI_Abort(comm, 1);
277
278     cp = N_VNew_Parallel(comm, local_N, SystemSize);
279     if(check_flag((void *)cp, "N_VNew_Parallel", 0, thispe)) MPI_Abort(comm, 1);
280
281     res = N_VNew_Parallel(comm, local_N, SystemSize);
282     if(check_flag((void *)res, "N_VNew_Parallel", 0, thispe)) MPI_Abort(comm, 1);
283
284     id = N_VNew_Parallel(comm, local_N, SystemSize);
285     if(check_flag((void *)id, "N_VNew_Parallel", 0, thispe)) MPI_Abort(comm, 1);
286
287     SetInitialProfiles(cc, cp, id, res, webdata);
288
289     N_VDestroy_Parallel(res);
290
291     /* Set remaining inputs to IDAMalloc. */
292
293     t0 = ZERO;

```

```

294     rtol = RTOL;
295     atol = ATOL;
296
297     /* Call IDACreate and IDAMalloc to initialize solution */
298
299     mem = IDACreate();
300     if(check_flag((void *)mem, "IDACreate", 0, thispe)) MPI_Abort(comm, 1);
301
302     retval = IDASetRdata(mem, webdata);
303     if(check_flag(&retval, "IDASetRdata", 1, thispe)) MPI_Abort(comm, 1);
304
305     retval = IDASetId(mem, id);
306     if(check_flag(&retval, "IDASetId", 1, thispe)) MPI_Abort(comm, 1);
307
308     retval = IDAMalloc(mem, resweb, t0, cc, cp, IDA_SS, rtol, &atol);
309     if(check_flag(&retval, "IDAMalloc", 1, thispe)) MPI_Abort(comm, 1);
310
311     /* Call IDABBDPrecAlloc to initialize the band-block-diagonal preconditioner.
312        The half-bandwidths for the difference quotient evaluation are exact
313        for the system Jacobian, but only a 5-diagonal band matrix is retained. */
314
315     mudq = mldq = NSMXSUB;
316     mukeep = mlkeep = 2;
317     P_data = IDABBDPrecAlloc(mem, local_N, mudq, mldq, mukeep, mlkeep,
318                             ZERO, reslocal, NULL);
319     if(check_flag((void *)P_data, "IDABBDPrecAlloc", 0, thispe)) MPI_Abort(comm, 1);
320
321     /* Call IDABBDSpgrmr to specify the IDA linear solver IDASPGMR and specify
322        the preconditioner routines supplied
323        maxl (max. Krylov subspace dim.) is set to 12.    */
324
325     maxl = 12;
326     retval = IDABBDSpgrmr(mem, maxl, P_data);
327     if(check_flag(&retval, "IDABBDSpgrmr", 1, thispe)) MPI_Abort(comm, 1);
328
329     /* Call IDACalcIC (with default options) to correct the initial values. */
330
331     tout = RCONST(0.001);
332     retval = IDACalcIC(mem, t0, cc, cp, IDA_YA_YDP_INIT, tout);
333     if(check_flag(&retval, "IDACalcIC", 1, thispe)) MPI_Abort(comm, 1);
334
335     /* On PE 0, print heading, basic parameters, initial values. */
336
337     if (thispe == 0) PrintHeader(SystemSize, maxl,
338                                 mudq, mldq, mukeep, mlkeep,
339                                 rtol, atol);
340     PrintOutput(mem, cc, t0, webdata, comm);
341
342     /* Call IDA in tout loop, normal mode, and print selected output. */
343
344     for (iout = 1; iout <= NOUT; iout++) {
345
346         retval = IDASolve(mem, tout, &tret, cc, cp, IDA_NORMAL);
347         if(check_flag(&retval, "IDASolve", 1, thispe)) MPI_Abort(comm, 1);
348
349         PrintOutput(mem, cc, tret, webdata, comm);
350
351         if (iout < 3) tout *= TMULT;
352         else           tout += TADD;

```

```

353     }
354
355     /* On PE 0, print final set of statistics. */
356
357     if (thispe == 0) PrintFinalStats(mem, P_data);
358
359     /* Free memory. */
360
361     N_VDestroy_Parallel(cc);
362     N_VDestroy_Parallel(cp);
363     N_VDestroy_Parallel(id);
364
365     IDABBDPrecFree(&P_data);
366
367     IDAFree(&mem);
368
369     denfree(webdata->acoef);
370     N_VDestroy_Parallel(webdata->rates);
371     free(webdata);
372
373     MPI_Finalize();
374
375     return(0);
376 }
377
378 /*
379 *-----*
380 * PRIVATE FUNCTIONS
381 *-----*
382 */
383
384 /*
385 * InitUserData: Load problem constants in webdata (of type UserData).
386 */
387
388 static void InitUserData(UserData webdata, int thispe, int npes,
389                         MPI_Comm comm)
390 {
391     int i, j, np;
392     realtype *a1,*a2, *a3, *a4, dx2, dy2, **acoef, *bcoef, *cox, *coy;
393
394     webdata->jysub = thispe / NPEX;
395     webdata->ixsub = thispe - (webdata->jysub)*NPEX;
396     webdata->mxsub = MXSUB;
397     webdata->mysub = MYSUB;
398     webdata->npex = NPEX;
399     webdata->npey = NPEY;
400     webdata->ns = NUM_SPECIES;
401     webdata->np = NPNEY;
402     webdata->dx = AX/(MX-1);
403     webdata->dy = AY/(MY-1);
404     webdata->thispe = thispe;
405     webdata->npes = npes;
406     webdata->nsmxsub = MXSUB * NUM_SPECIES;
407     webdata->nsmxsub2 = (MXSUB+2)*NUM_SPECIES;
408     webdata->comm = comm;
409     webdata->n_local = MXSUB*MYSUB*NUM_SPECIES;
410
411

```

```

412 /* Set up the coefficients a and b plus others found in the equations. */
413
414 np = webdata->np;
415 dx2 = (webdata->dx)*(webdata->dx);
416 dy2 = (webdata->dy)*(webdata->dy);
417
418 acoef = webdata->acoef;
419 bcoef = webdata->bcoef;
420 cox = webdata->cox;
421 coy = webdata->coy;
422
423 for (i = 0; i < np; i++) {
424     a1 = &(acoef[i][np]);
425     a2 = &(acoef[i+np][0]);
426     a3 = &(acoef[i][0]);
427     a4 = &(acoef[i+np][np]);
428     /* Fill in the portion of acoef in the four quadrants, row by row. */
429     for (j = 0; j < np; j++) {
430         *a1++ = -GG;
431         *a2++ = EE;
432         *a3++ = ZERO;
433         *a4++ = ZERO;
434     }
435
436     /* Reset the diagonal elements of acoef to -AA. */
437     acoef[i][i] = -AA; acoef[i+np][i+np] = -AA;
438
439     /* Set coefficients for b and diffusion terms. */
440     bcoef[i] = BB; bcoef[i+np] = -BB;
441     cox[i] = DPREY/dx2; cox[i+np] = DPRED/dx2;
442     coy[i] = DPREY/dy2; coy[i+np] = DPRED/dy2;
443 }
444
445 }
446
447 /*
448 * SetInitialProfiles: Set initial conditions in cc, cp, and id.
449 * A polynomial profile is used for the prey cc values, and a constant
450 * (1.0e5) is loaded as the initial guess for the predator cc values.
451 * The id values are set to 1 for the prey and 0 for the predators.
452 * The prey cp values are set according to the given system, and
453 * the predator cp values are set to zero.
454 */
455
456 static void SetInitialProfiles(N_Vector cc, N_Vector cp, N_Vector id,
457                               N_Vector res, UserData webdata)
458 {
459     long int ixsub, jysub, mxsub, mysub, nsmxsub, np, ix, jy, is;
460     realtype *cxy, *idxy, *cpxy, dx, dy, xx, yy, xyfactor;
461
462     ixsub = webdata->ixsub;
463     jysub = webdata->jysub;
464     mxsub = webdata->mxsub;
465     mysub = webdata->mxsub;
466     nsmxsub = webdata->nsmxsub;
467     dx = webdata->dx;
468     dy = webdata->dy;
469     np = webdata->np;
470

```

```

471 /* Loop over grid, load cc values and id values. */
472 for (jy = 0; jy < mysub; jy++) {
473     yy = (jy + jysub*mysub) * dy;
474     for (ix = 0; ix < mxsub; ix++) {
475         xx = (ix + ixsub*mxsub) * dx;
476         xyfactor = 16.*xx*(1. - xx)*yy*(1. - yy);
477         xyfactor *= xyfactor;
478
479         cxy = IJ_Vptr(cc, ix, jy);
480         idxy = IJ_Vptr(id, ix, jy);
481         for (is = 0; is < NUM_SPECIES; is++) {
482             if (is < np) { cxy[is] = RCONST(10.0) + (realtype)(is+1)*xyfactor; idxy[is] = ONE; }
483             else { cxy[is] = 1.0e5; idxy[is] = ZERO; }
484         }
485     }
486 }
487
488 /* Set c' for the prey by calling the residual function with cp = 0. */
489
490 N_VConst(ZERO, cp);
491 resweb(ZERO, cc, cp, res, webdata);
492 N_VScale(-ONE, res, cp);
493
494 /* Set c' for predators to 0. */
495
496 for (jy = 0; jy < mysub; jy++) {
497     for (ix = 0; ix < mxsub; ix++) {
498         cpvy = IJ_Vptr(cp, ix, jy);
499         for (is = np; is < NUM_SPECIES; is++) cpvy[is] = ZERO;
500     }
501 }
502 }
503
504 /*
505 * Print first lines of output (problem description)
506 * and table header
507 */
508
509 static void PrintHeader(long int SystemSize, int maxl,
510                         long int mudq, long int mldq,
511                         long int mukeep, long int mlkeep,
512                         realtype rtol, realtype atol)
513 {
514     printf("\nidakryx2_bbd_p: Predator-prey DAE parallel example problem\n\n");
515     printf("Number of species: %d\n", NUM_SPECIES);
516     printf("Mesh dimensions: %d x %d\n", MX, MY);
517     printf("Total system size: %ld\n", SystemSize);
518     printf("Subgrid dimensions: %d x %d\n", MXSUB, MYSUB);
519     printf("Processor array: %d x %d\n", NPEX, NPEY);
520     printf("Tolerance parameters:\n");
521 #if defined(SUNDIALS_EXTENDED_PRECISION)
522     printf(" relative tolerance = %Lg\n", rtol);
523     printf(" absolute tolerance = %Lg\n", atol);
524 #elif defined(SUNDIALS_DOUBLE_PRECISION)
525     printf(" relative tolerance = %lg\n", rtol);
526     printf(" absolute tolerance = %lg\n", atol);
527 #else
528     printf(" relative tolerance = %g\n", rtol);
529     printf(" absolute tolerance = %g\n", atol);

```

```

530 #endif
531 printf("Linear solver: scaled preconditioned GMRES (IDASPGMR)\n");
532 printf(" max. Krylov dimension: maxl = %d\n", maxl);
533 printf("Preconditioner: band-block-diagonal (IDABBDPRE)\n");
534 printf(" mudq = %ld, mldq = %ld, mukeep = %ld, mlkeep = %ld\n",
535     mudq, mldq, mukeep, mlkeep);
536 printf("CalcIC called to correct initial predator concentrations\n\n");
537 printf("-----\n");
538 printf("ut bottom-left top-right");
539 printf("nst kuh\n");
540 printf("-----\n\n");
541 }
542
543
544 /*
545 * PrintOutput: Print output values at output time t = tt.
546 * Selected run statistics are printed. Then values of c1 and c2
547 * are printed for the bottom left and top right grid points only.
548 */
549
550 static void PrintOutput(void *mem, N_Vector cc, realtype tt,
551                         UserData webdata, MPI_Comm comm)
552 {
553     MPI_Status status;
554     realtype *cdata, clast[2], hused;
555     long int nst;
556     int i, kused, flag, thispe, npelast, ilast;;
557
558     thispe = webdata->thispe;
559     npelast = webdata->nipes - 1;
560     cdata = NV_DATA_P(cc);
561
562     /* Send conc. at top right mesh point from PE nipes-1 to PE 0. */
563     if (thispe == npelast) {
564         ilast = NUM_SPECIES*MXSUB*MYSUB - 2;
565         if (npelast != 0)
566             MPI_Send(&cdata[ilast], 2, PVEC_REAL_MPI_TYPE, 0, 0, comm);
567         else { clast[0] = cdata[ilast]; clast[1] = cdata[ilast+1]; }
568     }
569
570     /* On PE 0, receive conc. at top right from PE nipes - 1.
571        Then print performance data and sampled solution values. */
572
573     if (thispe == 0) {
574
575         if (npelast != 0)
576             MPI_Recv(&clast[0], 2, PVEC_REAL_MPI_TYPE, npelast, 0, comm, &status);
577
578         flag = IDAGetLastOrder(mem, &kused);
579         check_flag(&flag, "IDAGetLastOrder", 1, thispe);
580         flag = IDAGetNumSteps(mem, &nst);
581         check_flag(&flag, "IDAGetNumSteps", 1, thispe);
582         flag = IDAGetLastStep(mem, &hused);
583         check_flag(&flag, "IDAGetLastStep", 1, thispe);
584
585     #if defined(SUNDIALS_EXTENDED_PRECISION)
586         printf("%8.2Le%12.4Le%12.4Le| %3ld%1d%12.4Le\n",
587                tt, cdata[0], clast[0], nst, kused, hused);
588         for (i=1;i<NUM_SPECIES;i++)

```

```

589     printf("uuuuuuuuuu%12.4Le%12.4Leuuu|\n", cdata[i], clast[i]);
590 #elif defined(SUNDIALS_DOUBLE_PRECISION)
591     printf("%8.2le%12.4le%12.4leuuu|u%3lduu%1d%12.4le\n",
592            tt, cdata[0], clast[0], nst, kused, hused);
593     for (i=1;i<NUM_SPECIES;i++)
594         printf("uuuuuuuuuu%12.4le%12.4leuuu|\n", cdata[i], clast[i]);
595 #else
596     printf("%8.2e%12.4e%12.4euuu|u%3lduu%1d%12.4e\n",
597            tt, cdata[0], clast[0], nst, kused, hused);
598     for (i=1;i<NUM_SPECIES;i++)
599         printf("uuuuuuuuuu%12.4e%12.4euuu|\n", cdata[i], clast[i]);
600 #endif
601     printf("\n");
602
603 }
604
605 }
606
607 /*
608 * PrintFinalStats: Print final run data contained in iopt.
609 */
610
611 static void PrintFinalStats(void *mem, void *P_data)
612 {
613     long int nst, nre, nreLS, netf, ncfn, nni, ncfl, nli, npe, nps, nge;
614     int flag;
615
616     flag = IDAGetNumSteps(mem, &nst);
617     check_flag(&flag, "IDAGetNumSteps", 1, 0);
618     flag = IDAGetNumResEvals(mem, &nre);
619     check_flag(&flag, "IDAGetNumResEvals", 1, 0);
620     flag = IDAGetNumErrTestFails(mem, &netf);
621     check_flag(&flag, "IDAGetNumErrTestFails", 1, 0);
622     flag = IDAGetNumNonlinSolvConvFails(mem, &ncfn);
623     check_flag(&flag, "IDAGetNumNonlinSolvConvFails", 1, 0);
624     flag = IDAGetNumNonlinSolvIterers(mem, &nni);
625     check_flag(&flag, "IDAGetNumNonlinSolvIterers", 1, 0);
626
627     flag = IDASpilsGetNumConvFails(mem, &ncfl);
628     check_flag(&flag, "IDASpilsGetNumConvFails", 1, 0);
629     flag = IDASpilsGetNumLinIterers(mem, &nli);
630     check_flag(&flag, "IDASpilsGetNumLinIterers", 1, 0);
631     flag = IDASpilsGetNumPrecEvals(mem, &npe);
632     check_flag(&flag, "IDASpilsGetNumPrecEvals", 1, 0);
633     flag = IDASpilsGetNumPrecSolves(mem, &nps);
634     check_flag(&flag, "IDASpilsGetNumPrecSolves", 1, 0);
635     flag = IDASpilsGetNumResEvals(mem, &nreLS);
636     check_flag(&flag, "IDASpilsGetNumResEvals", 1, 0);
637
638     flag = IDABBDPrecGetNumGfnEvals(P_data, &nge);
639     check_flag(&flag, "IDABBDPrecGetNumGfnEvals", 1, 0);
640
641     printf("-----\n");
642     printf("\nFinal statistics:\n\n");
643
644     printf("Number of steps = %ld\n", nst);
645     printf("Number of residual evaluations = %ld\n", nre+nreLS);
646     printf("Number of nonlinear iterations = %ld\n", nni);
647     printf("Number of error test failures = %ld\n", netf);

```

```

648 printf("Number of nonlinear conv. failures = %ld\n\n", ncfn);
649
650 printf("Number of linear iterations = %ld\n", nli);
651 printf("Number of linear conv. failures = %ld\n\n", ncfl);
652
653 printf("Number of preconditioner setups = %ld\n", npe);
654 printf("Number of preconditioner solves = %ld\n", nps);
655 printf("Number of local residual evals. = %ld\n", nge);
656
657 }
658
659 /*
660 * Check function return value...
661 *   opt == 0 means SUNDIALS function allocates memory so check if
662 *           returned NULL pointer
663 *   opt == 1 means SUNDIALS function returns a flag so check if
664 *           flag >= 0
665 *   opt == 2 means function allocates memory so check if returned
666 *           NULL pointer
667 */
668
669 static int check_flag(void *flagvalue, char *funcname, int opt, int id)
670 {
671     int *errflag;
672
673     if (opt == 0 && flagvalue == NULL) {
674         /* Check if SUNDIALS function returned NULL pointer - no memory allocated */
675         fprintf(stderr,
676                 "\nSUNDIALS_ERROR(%d): %s() failed - returned NULL pointer\n\n",
677                 id, funcname);
678         return(1);
679     } else if (opt == 1) {
680         /* Check if flag < 0 */
681         errflag = (int *) flagvalue;
682         if (*errflag < 0) {
683             fprintf(stderr,
684                     "\nSUNDIALS_ERROR(%d): %s() failed with flag = %d\n\n",
685                     id, funcname, *errflag);
686             return(1);
687         }
688     } else if (opt == 2 && flagvalue == NULL) {
689         /* Check if function returned NULL pointer - no memory allocated */
690         fprintf(stderr,
691                 "\nMEMORY_ERROR(%d): %s() failed - returned NULL pointer\n\n",
692                 id, funcname);
693         return(1);
694     }
695
696     return(0);
697 }
698
699 /*
700 *-----*
701 * FUNCTIONS CALLED BY IDA & SUPPORTING FUNCTIONS
702 *-----*
703 */
704
705 /*
706 * resweb: System residual function for predator-prey system.

```

```

707 * To compute the residual function F, this routine calls:
708 * rescomm, for needed communication, and then
709 * reslocal, for computation of the residuals on this processor.
710 */
711
712 static int resweb(realtytype tt,
713                     N_Vector cc, N_Vector cp, N_Vector rr,
714                     void *res_data)
715 {
716     int retval;
717     UserData webdata;
718     long int Nlocal;
719
720     webdata = (UserData) res_data;
721
722     Nlocal = webdata->n_local;
723
724     /* Call rescomm to do inter-processor communication. */
725     retval = rescomm(Nlocal, tt, cc, cp, res_data);
726
727     /* Call reslocal to calculate the local portion of residual vector. */
728     retval = reslocal(Nlocal, tt, cc, cp, rr, res_data);
729
730     return(0);
731 }
732
733 /*
734 * rescomm: Communication routine in support of resweb.
735 * This routine performs all inter-processor communication of components
736 * of the cc vector needed to calculate F, namely the components at all
737 * interior subgrid boundaries (ghost cell data). It loads this data
738 * into a work array cext (the local portion of c, extended).
739 * The message-passing uses blocking sends, non-blocking receives,
740 * and receive-waiting, in routines BRecvPost, BSend, BRecvWait.
741 */
742
743 static int rescomm(long int Nlocal, realtytype tt,
744                     N_Vector cc, N_Vector cp,
745                     void *res_data)
746 {
747
748     UserData webdata;
749     realtype *cdata, *cext, buffer[2*NUM_SPECIES*MYSUB];
750     long int thispe, ixsub, jysub, nsmxsub, nsmysub;
751     MPI_Comm comm;
752     MPI_Request request[4];
753
754     webdata = (UserData) res_data;
755     cdata = NV_DATA_P(cc);
756
757     /* Get comm, thispe, subgrid indices, data sizes, extended array cext. */
758
759     comm = webdata->comm;
760     thispe = webdata->thispe;
761
762     ixsub = webdata->ixsub;
763     jysub = webdata->jysub;
764     cext = webdata->cext;
765     nsmxsub = webdata->nsmxsub;

```

```

766 nsmysub = (webdata->ns)*(webdata->mysub);
767
768 /* Start receiving boundary data from neighboring PEs. */
769
770 BRecvPost(comm, request, thispe, ixsub, jysub, nsmxsub, nsmysub,
771 cext, buffer);
772
773 /* Send data from boundary of local grid to neighboring PEs. */
774
775 BSend(comm, thispe, ixsub, jysub, nsmxsub, nsmysub, cdata);
776
777 /* Finish receiving boundary data from neighboring PEs. */
778
779 BRecvWait(request, ixsub, jysub, nsmxsub, cext, buffer);
780
781 return(0);
782 }
783
784 /*
785 * BRecvPost: Start receiving boundary data from neighboring PEs.
786 * (1) buffer should be able to hold 2*NUM_SPECIES*MYSUB realltype entries,
787 *      should be passed to both the BRecvPost and BRecvWait functions, and
788 *      should not be manipulated between the two calls.
789 * (2) request should have 4 entries, and is also passed in both calls.
790 */
791
792 static void BRecvPost(MPI_Comm comm, MPI_Request request[], long int my_pe,
793                      long int ixsub, long int jysub,
794                      long int dsizex, long int dsizey,
795                      realltype cext[], realltype buffer[])
796 {
797     long int offsetce;
798     /* Have bufleft and bufright use the same buffer. */
799     realltype *bufleft = buffer, *bufright = buffer+NUM_SPECIES*MYSUB;
800
801     /* If jysub > 0, receive data for bottom x-line of cext. */
802     if (jysub != 0)
803         MPI_Irecv(&cext[NUM_SPECIES], dsizex, PVEC_REAL_MPI_TYPE,
804                   my_pe-NPEX, 0, comm, &request[0]);
805
806     /* If jysub < NPEY-1, receive data for top x-line of cext. */
807     if (jysub != NPEY-1) {
808         offsetce = NUM_SPECIES*(1 + (MYSUB+1)*(MXSUB+2));
809         MPI_Irecv(&cext[offsetce], dsizex, PVEC_REAL_MPI_TYPE,
810                   my_pe+NPEX, 0, comm, &request[1]);
811     }
812
813     /* If ixsub > 0, receive data for left y-line of cext (via bufleft). */
814     if (ixsub != 0) {
815         MPI_Irecv(&bufleft[0], dsizey, PVEC_REAL_MPI_TYPE,
816                   my_pe-1, 0, comm, &request[2]);
817     }
818
819     /* If ixsub < NPEX-1, receive data for right y-line of cext (via bufright). */
820     if (ixsub != NPEX-1) {
821         MPI_Irecv(&bufright[0], dsizey, PVEC_REAL_MPI_TYPE,
822                   my_pe+1, 0, comm, &request[3]);
823     }
824

```

```

825 }
826
827 /*
828 * BRecvWait: Finish receiving boundary data from neighboring PEs.
829 * (1) buffer should be able to hold 2*NUM_SPECIES*MYSUB realtype entries,
830 *      should be passed to both the BRecvPost and BRecvWait functions, and
831 *      should not be manipulated between the two calls.
832 * (2) request should have 4 entries, and is also passed in both calls.
833 */
834
835 static void BRecvWait(MPI_Request request[], long int ixsub, long int jysub,
836                      long int dsizex, realtype cext[], realtype buffer[])
837 {
838     int i;
839     long int ly, dsizex2, offsetce, offsetbuf;
840     realtype *bufleft = buffer, *bufright = buffer+NUM_SPECIES*MYSUB;
841     MPI_Status status;
842
843     dsizex2 = dsizex + 2*NUM_SPECIES;
844
845     /* If jysub > 0, receive data for bottom x-line of cext. */
846     if (jysub != 0)
847         MPI_Wait(&request[0],&status);
848
849     /* If jysub < NPEY-1, receive data for top x-line of cext. */
850     if (jysub != NPEY-1)
851         MPI_Wait(&request[1],&status);
852
853     /* If ixsub > 0, receive data for left y-line of cext (via bufleft). */
854     if (ixsub != 0) {
855         MPI_Wait(&request[2],&status);
856
857         /* Copy the buffer to cext */
858         for (ly = 0; ly < MYSUB; ly++) {
859             offsetbuf = ly*NUM_SPECIES;
860             offsetce = (ly+1)*dsizex2;
861             for (i = 0; i < NUM_SPECIES; i++)
862                 cext[offsetce+i] = bufleft[offsetbuf+i];
863         }
864     }
865
866     /* If ixsub < NPEX-1, receive data for right y-line of cext (via bufright). */
867     if (ixsub != NPEX-1) {
868         MPI_Wait(&request[3],&status);
869
870         /* Copy the buffer to cext */
871         for (ly = 0; ly < MYSUB; ly++) {
872             offsetbuf = ly*NUM_SPECIES;
873             offsetce = (ly+2)*dsizex2 - NUM_SPECIES;
874             for (i = 0; i < NUM_SPECIES; i++)
875                 cext[offsetce+i] = bufright[offsetbuf+i];
876         }
877     }
878 }
879
880 /*
881 * BSend: Send boundary data to neighboring PEs.
882 * This routine sends components of cc from internal subgrid boundaries
883 * to the appropriate neighbor PEs.

```

```

884     */
885
886 static void BSend(MPI_Comm comm, long int my_pe, long int ixsub, long int jysub,
887                   long int dsizex, long int dsizey, realtype cdata[])
888 {
889     int i;
890     long int ly, offsetc, offsetbuf;
891     realtype bufleft[NUM_SPECIES*MYSUB], bufright[NUM_SPECIES*MYSUB];
892
893     /* If jysub > 0, send data from bottom x-line of cc. */
894
895     if (jysub != 0)
896         MPI_Send(&cdata[0], dsizex, PVEC_REAL_MPI_TYPE, my_pe-NPEX, 0, comm);
897
898     /* If jysub < NPEY-1, send data from top x-line of cc. */
899
900     if (jysub != NPEY-1) {
901         offsetc = (MYSUB-1)*dsizex;
902         MPI_Send(&cdata[offsetc], dsizex, PVEC_REAL_MPI_TYPE, my_pe+NPEX, 0, comm);
903     }
904
905     /* If ixsub > 0, send data from left y-line of cc (via bufleft). */
906
907     if (ixsub != 0) {
908         for (ly = 0; ly < MYSUB; ly++) {
909             offsetbuf = ly*NUM_SPECIES;
910             offsetc = ly*dsizex;
911             for (i = 0; i < NUM_SPECIES; i++)
912                 bufleft[offsetbuf+i] = cdata[offsetc+i];
913         }
914         MPI_Send(&bufleft[0], dsizey, PVEC_REAL_MPI_TYPE, my_pe-1, 0, comm);
915     }
916
917     /* If ixsub < NPEX-1, send data from right y-line of cc (via bufright). */
918
919     if (ixsub != NPEX-1) {
920         for (ly = 0; ly < MYSUB; ly++) {
921             offsetbuf = ly*NUM_SPECIES;
922             offsetc = offsetbuf*MYSUB + (MYSUB-1)*NUM_SPECIES;
923             for (i = 0; i < NUM_SPECIES; i++)
924                 bufright[offsetbuf+i] = cdata[offsetc+i];
925         }
926         MPI_Send(&bufright[0], dsizey, PVEC_REAL_MPI_TYPE, my_pe+1, 0, comm);
927     }
928 }
929
930 /* Define lines are for ease of readability in the following functions. */
931
932 #define mxsub      (webdata->mxsub)
933 #define mysub      (webdata->mysub)
934 #define npex       (webdata->npex)
935 #define npey       (webdata->npey)
936 #define ixsub      (webdata->ixsub)
937 #define jysub      (webdata->jysub)
938 #define nsmxsub    (webdata->nsmxsub)
939 #define nsmxsub2   (webdata->nsmxsub2)
940 #define np        (webdata->np)
941 #define dx        (webdata->dx)
942 #define dy        (webdata->dy)

```

```

943 #define cox      (webdata->cox)
944 #define coy      (webdata->coy)
945 #define rhs      (webdata->rhs)
946 #define cext     (webdata->cext)
947 #define rates    (webdata->rates)
948 #define ns       (webdata->ns)
949 #define acoef    (webdata->acoef)
950 #define bcoef    (webdata->bcoef)
951
952 /*
953 * reslocal: Compute res = F(t,cc,cp).
954 * This routine assumes that all inter-processor communication of data
955 * needed to calculate F has already been done. Components at interior
956 * subgrid boundaries are assumed to be in the work array cext.
957 * The local portion of the cc vector is first copied into cext.
958 * The exterior Neumann boundary conditions are explicitly handled here
959 * by copying data from the first interior mesh line to the ghost cell
960 * locations in cext. Then the reaction and diffusion terms are
961 * evaluated in terms of the cext array, and the residuals are formed.
962 * The reaction terms are saved separately in the vector webdata->rates
963 * for use by the preconditioner setup routine.
964 */
965
966 static int reslocal(long int Nlocal, realtype tt,
967                      N_Vector cc, N_Vector cp, N_Vector rr,
968                      void *res_data)
969 {
970     realtype *cdata, *ratesxy, *cpxy, *resxy,
971     xx, yy, dcyli, dcui, dcxli, dcxui;
972     long int ix, jy, is, i, locc, ylocce, locce;
973     UserData webdata;
974
975     webdata = (UserData) res_data;
976
977     /* Get data pointers, subgrid data, array sizes, work array cext. */
978
979     cdata = NV_DATA_P(cc);
980
981     /* Copy local segment of cc vector into the working extended array cext. */
982
983     locc = 0;
984     locce = nsmxsub2 + NUM_SPECIES;
985     for (jy = 0; jy < mysub; jy++) {
986         for (i = 0; i < nsmxsub; i++) cext[locc+i] = cdata[locc+i];
987         locc = locc + nsmxsub;
988         locce = locce + nsmxsub2;
989     }
990
991     /* To facilitate homogeneous Neumann boundary conditions, when this is
992        a boundary PE, copy data from the first interior mesh line of cc to cext. */
993
994     /* If jysub = 0, copy x-line 2 of cc to cext. */
995     if (jysub == 0)
996         { for (i = 0; i < nsmxsub; i++) cext[NUM_SPECIES+i] = cdata[nsmxsub+i]; }
997
998     /* If jysub = npey-1, copy x-line mysub-1 of cc to cext. */
999     if (jysub == npey-1) {
1000         locc = (mysub-2)*nsmxsub;
1001         locce = (mysub+1)*nsmxsub2 + NUM_SPECIES;

```

```

1002     for (i = 0; i < nsmxsub; i++) cext[locce+i] = cdata[locc+i];
1003 }
1004
1005 /* If ixsub = 0, copy y-line 2 of cc to cext. */
1006 if (ixsub == 0) {
1007     for (jy = 0; jy < mysub; jy++) {
1008         locc = jy*nsmxsub + NUM_SPECIES;
1009         locce = (jy+1)*nsmxsub2;
1010         for (i = 0; i < NUM_SPECIES; i++) cext[locce+i] = cdata[locc+i];
1011     }
1012 }
1013
1014 /* If ixsub = npex-1, copy y-line mbsub-1 of cc to cext. */
1015 if (ixsub == npex-1) {
1016     for (jy = 0; jy < mysub; jy++) {
1017         locc = (jy+1)*nsmxsub - 2*NUM_SPECIES;
1018         locce = (jy+2)*nsmxsub2 - NUM_SPECIES;
1019         for (i = 0; i < NUM_SPECIES; i++) cext[locce+i] = cdata[locc+i];
1020     }
1021 }
1022
1023 /* Loop over all grid points, setting local array rates to right-hand sides.
1024    Then set rr values appropriately for prey/predator components of F. */
1025
1026 for (jy = 0; jy < mysub; jy++) {
1027     ylocce = (jy+1)*nsmxsub2;
1028     yy      = (jy+jysub*mysub)*dy;
1029
1030     for (ix = 0; ix < mxsub; ix++) {
1031         locce = ylocce + (ix+1)*NUM_SPECIES;
1032         xx   = (ix + ixsub*mxsub)*dx;
1033
1034         ratesxy = IJ_Vptr(rates, ix, jy);
1035         WebRates(xx, yy, &(cext[locce]), ratesxy, webdata);
1036
1037         resxy = IJ_Vptr(rr, ix, jy);
1038         cpxy = IJ_Vptr(cp, ix, jy);
1039
1040         for (is = 0; is < NUM_SPECIES; is++) {
1041             dcycli = cext[locce+is]           - cext[locce+is-nsmxsub2];
1042             dcuyi = cext[locce+is+nsmxsub2] - cext[locce+is];
1043
1044             dcxli = cext[locce+is]           - cext[locce+is-NUM_SPECIES];
1045             dcxui = cext[locce+is+NUM_SPECIES] - cext[locce+is];
1046
1047             rhs[is] = cox[is]*(dcxui-dcxli) + coy[is]*(dcuyi-dcycli) + ratesxy[is];
1048
1049             if (is < np) resxy[is] = cpxy[is] - rhs[is];
1050             else        resxy[is] =          - rhs[is];
1051
1052         }
1053     }
1054 }
1055
1056 return(0);
1057 }
1058
1059 /*
1060 * WebRates: Evaluate reaction rates at a given spatial point.

```

```

1061 * At a given (x,y), evaluate the array of ns reaction terms R.
1062 */
1063
1064 static void WebRates(realtype xx, realtype yy, realtype *cxy, realtype *ratesxy,
1065                      UserData webdata)
1066 {
1067     int is;
1068     realtype fac;
1069
1070     for (is = 0; is < NUM_SPECIES; is++)
1071         ratesxy[is] = dotprod(NUM_SPECIES, cxy, acoef[is]);
1072
1073     fac = ONE + ALPHA*xx*yy + BETA*sin(FOURPI*xx)*sin(FOURPI*yy);
1074
1075     for (is = 0; is < NUM_SPECIES; is++)
1076         ratesxy[is] = cxy[is]*( bcoef[is]*fac + ratesxy[is] );
1077
1078 }
1079
1080 /*
1081 * dotprod: dot product routine for realtype arrays, for use by WebRates.
1082 */
1083
1084 static realtype dotprod(long int size, realtype *x1, realtype *x2)
1085 {
1086     long int i;
1087     realtype *xx1, *xx2, temp = ZERO;
1088
1089     xx1 = x1;
1090     xx2 = x2;
1091     for (i = 0; i < size; i++)
1092         temp += (*xx1++) * (*xx2++);
1093
1094     return(temp);
1095 }
1096

```

F Listing of fidadenx.f

```
1  c  -----
2  c  $Revision: 1.5 $
3  c  $Date: 2006/03/24 00:28:51 $
4  c  -----
5  c  This simple example problem for FIDA, due to Robertson, is from
6  c  chemical kinetics, and consists of the following three equations:
7  c
8  c      dy1/dt = -.04*y1 + 1.e4*y2*y3
9  c      dy2/dt = .04*y1 - 1.e4*y2*y3 - 3.e7*y2**2
10 c      0     = y1 + y2 + y3 - 1
11 c
12 c  on the interval from t = 0.0 to t = 4.e10, with initial
13 c  conditions: y1 = 1, y2 = y3 = 0.
14 c
15 c  While integrating the system, we also use the rootfinding feature
16 c  to find the points at which y1 = 1.e-4 or at which y3 = 0.01.
17 c
18 c  The problem is solved using a dense linear solver, with a
19 c  user-supplied Jacobian. Output is printed at
20 c  t = .4, 4, 40, ..., 4e10.
21 c  -----
22 c
23 program fidadenx
24 c
25 implicit none
26 c
27 integer ier, ierroot, info(2)
28 integer*4 iout(25), ipar
29 double precision rout(10), rpar
30 c
31 integer iatol, nout, jout, itask
32 integer nst, kused, hused
33 integer*4 neq, i
34 double precision t0, t1, rtol, tout, tret
35 double precision y(3), yp(3), atol(3)
36 c
37 data nst/3/, kused/9/, hused/2/
38 c
39 c Initialize variables
40 c
41 neq = 3
42 nout = 12
43 rtol = 1.0d-4
44 t0 = 0.0d0
45 t1 = 0.4d0
46 iatol = 2
47 itask = 1
48 c
49 y(1) = 1.0d0
50 y(2) = 0.0d0
51 y(3) = 0.0d0
52 c
53 yp(1) = -0.04d0
54 yp(2) = 0.04d0
55 yp(3) = 0.0d0
56 c
57 atol(1) = 1.0d-6
```

```

58         atol(2) = 1.0d-10
59         atol(3) = 1.0d-6
60
61 c Initialize IDA vector environment
62
63     call fnvinit(2, neq, ier)
64     if (ier .ne. 0) then
65         write(6,10) ier
66     10      format(///' SUNDIALS_ERROR: FNVINIT returned IER = ', i5)
67         stop
68     endif
69
70     call fidamalloc(t0, y, yp, iatol, rtol, atol,
71 &                      iout, rout, ipar, rpar, ier)
72     if (ier .ne. 0) then
73         write(6,20) ier
74     20      format(///' SUNDIALS_ERROR: FIDAMALLOC returned IER = ', i5)
75         stop
76     endif
77
78 c Initialize rootfinding problem
79
80     call fidarootinit(2, ier)
81     if (ier .ne. 0) then
82         write(6,25) ier
83     25      format(///' SUNDIALS_ERROR: FIDAROOTINIT returned IER = ', i5)
84         call fidafree
85         stop
86     endif
87
88 c Attach dense linear solver
89
90     call fidadense(neq, ier)
91     call fidadensesetjac(1, ier)
92
93 c Print header
94
95     call prntintro(rtol, atol, y)
96
97     tout = t1
98
99
100    jout = 1
101    do while(jout .le. nout)
102
103        call fidasolve(tout, tret, y, yp, itask, ier)
104
105        write(6,40) tret, (y(i), i = 1,3), iout(nst), iout(kused),
106 &                      rout(hused)
107    40      format(e10.4, 3(1x,e12.4), i5, i3, e12.4)
108
109        if (ier .lt. 0) then
110            write(6,50) ier, iout(15)
111    50      format(///' SUNDIALS_ERROR: FIDASOLVE returned IER = ',i5,/,
112           1                           '                               Linear Solver returned IER = ',i5)
113            call fidarootfree
114            call fidafree
115            stop
116        endif

```

```

117  c
118      if (ier .eq. 2) then
119          call fidarootinfo(2, info, ierroot)
120          if (ierroot .lt. 0) then
121              write(6,55) ier
122          55      format(///' SUNDIALS_ERROR: FIDAROOTINFO returned IER = ',
123              1                  i5)
124          call fidarootfree
125          call fidafree
126          stop
127          endif
128          write(6,60) (info(i), i = 1,2)
129          60      format(5x, 'Above is a root, INFO() = ', 2i3)
130          endif
131  c
132      if (ier .eq. 0) then
133          tout = tout * 10.0d0
134          jout = jout + 1
135          endif
136  c
137      ENDDO
138  c
139  c Print final statistics
140  c
141      call prntstats(iout)
142  c
143  c Free IDA memory
144  c
145      call fidarootfree
146      call fidafree
147  c
148      stop
149      end
150  c
151  c ======
152  c
153      subroutine fidaresfun(tres, y, yp, res, ipar, rpar, reserr)
154  c
155      implicit none
156  c
157      integer reserr
158      integer*4 ipar(*)
159      double precision tres, rpar(*)
160      double precision y(*), yp(*), res(*)
161  c
162      res(1) = -0.04d0*y(1)+1.0d4*y(2)*y(3)
163      res(2) = -res(1)-3.0d7*y(2)*y(2)-yp(2)
164      res(1) = res(1)-yp(1)
165      res(3) = y(1)+y(2)+y(3)-1.0d0
166  c
167      reserr = 0
168  c
169      return
170      end
171  c
172  c ======
173  c
174      subroutine fidadjac(neq, t, y, yp, r, jac, cj, ewt, h,
175          1                  ipar, rpar, wk1, wk2, wk3, djacerr)

```

```

176  c
177      implicit none
178  c
179      integer*4 neq, ipar(*)
180      integer djacerr
181      double precision t, h, cj, rpar(*)
182      double precision y(*), yp(*), r(*), ewt(*), jac(neq,neq)
183      double precision wk1(*), wk2(*), wk3(*)
184  c
185      jac(1,1) = -0.04d0-cj
186      jac(2,1) = 0.04d0
187      jac(3,1) = 1.0d0
188      jac(1,2) = 1.0d4*y(3)
189      jac(2,2) = -1.0d4*y(3)-6.0d7*y(2)-cj
190      jac(3,2) = 1.0d0
191      jac(1,3) = 1.0d4*y(2)
192      jac(2,3) = -1.0d4*y(2)
193      jac(3,3) = 1.0d0
194  c
195      djacerr = 0
196
197      return
198  end
199  c
200  c =====
201  c
202      subroutine fidarootfn(t, y, yp, g, ipar, rpar, ier)
203  c Fortran routine for rootfinding
204      implicit none
205  c
206      INTEGER*4 ipar(*), ier
207      double precision t, y(*), yp(*), g(*), rpar(*)
208  c
209      g(1) = y(1) - 1.0d-4
210      g(2) = y(3) - 1.0d-2
211
212      ier = 0
213
214      return
215  end
216  c
217  c =====
218  c
219      subroutine prntintro(rtol, atol, y)
220  c
221      implicit none
222  c
223      integer*4 i
224      double precision rtol, atol(*), y(*)
225  c
226      write(6,60) rtol, (atol(i), i = 1,3), (y(i), i = 1,3)
227  60      format(/'fidadenx: Robertson kinetics DAE serial example',
228      &           'problem for IDA', /,'                                Three equation chemical',
229      &           'kinetics problem.', //,
230      &           'Tolerance parameters: rtol = ', e8.2,
231      &           '      atol = ', 3(1x,e8.2), /,
232      &           'Initial conditions y0 = (', 3(1x,e8.2), ')', //,
233      &           '      t                  y1                  y2                  y3      nst',
234      &           '      k      h')

```

```

235   C
236       return
237   end
238   C
239   C =====
240   C
241       subroutine prntstats(iout)
242   C
243       implicit none
244   C
245       integer*4 iout(25)
246       integer nst, reseval, jaceval, nni, ncf, netf, nge
247   C
248       data nst/3/, reseval/4/, jaceval/17/, nni/7/, netf/5/,
249       &      ncf/6/, nge/12/
250   C
251       write(6,70) iout(nst), iout(reseval), iout(jaceval),
252       &          iout(nni), iout(netf), iout(ncf), iout(nge)
253   70    format(/'Final Run Statistics:', //,
254       &          'Number of steps                  = ', i3, '/',
255       &          'Number of residual evaluations   = ', i3, '/',
256       &          'Number of Jacobian evaluations  = ', i3, '/',
257       &          'Number of nonlinear iterations   = ', i3, '/',
258       &          'Number of error test failures   = ', i3, '/',
259       &          'Number of nonlinear conv. failures = ', i3, '/',
260       &          'Number of root function evals.  = ', i3)
261   C
262       return
263   end

```

G Listing of fidakryx_bbd_p.f

```
1  c  -----
2  c  $Revision: 1.3 $
3  c  $Date: 2006/01/24 22:17:31 $
4  c  -----
5  c  Example problem for FIDA: 2D heat equation, parallel, GMRES,
6  c  IDABBDPRE.
7  c
8  c  This example solves a discretized 2D heat equation problem.
9  c  This version uses the Krylov solver IDASPGMR and BBD
10 c  preconditioning.
11 c
12 c  The DAE system solved is a spatial discretization of the PDE
13 c  du/dt = d^2u/dx^2 + d^2u/dy^2
14 c  on the unit square. The boundary condition is u = 0 on all edges.
15 c  Initial conditions are given by u = 16 x (1 - x) y (1 - y). The
16 c  PDE is treated with central differences on a uniform MX x MY
17 c  grid. The values of u at the interior points satisfy ODEs, and
18 c  equations u = 0 at the boundaries are appended, to form a DAE
19 c  system of size N = MX * MY. Here MX = MY = 10.
20 c
21 c  The system is actually implemented on submeshes, processor by
22 c  processor, with an MXSUB by MYSUB mesh on each of NPEX * NPEY
23 c  processors.
24 c
25 c  The system is solved with FIDA using the Krylov linear solver
26 c  IDASPGMR in conjunction with the preconditioner module IDABBDPRE.
27 c  The preconditioner uses a tridiagonal approximation
28 c  (half-bandwidths = 1). The constraints u >= 0 are posed for all
29 c  components. Local error testing on the boundary values is
30 c  suppressed. Output is taken at t = 0, .01, .02, .04, ..., 10.24.
31 c  -----
32 c
33 program fidakryx_bbd_p
34 c
35 include "mpif.h"
36 c
37 c global variables
38 c
39 integer*4 nlocal, neq, npex, npey, mxsub, mysub, mx, my
40 integer*4 ixsub, jysub
41 integer thispe
42 integer mxsubg, mysubg, nlocalg
43 parameter (mxsubg = 5, mysubg = 5)
44 parameter (nlocalg = mxsubg*mysubg)
45 double precision dx, dy, coeffx, coeffy, coeffxy
46 double precision uext((mxsubg+2)*(mysubg+2))
47 c
48 c local variables
49 c
50 integer*4 mudq, mldq, mukeep, mlkeep
51 integer*4 iout(25), ipar
52 double precision rout(10), rpar
53 integer nout, ier
54 parameter (nout = 11)
55 integer npes, inopt, maxl, gstype, maxrs, itask, iatol
56 double precision t0, t1, tout, tret, dqrely, eplifac, dqincfac
57 double precision atol, rtol
```

```

58      double precision constr(nlocalg), uu(nlocalg), up(nlocalg)
59      double precision res(nlocalg), id(nlocalg)
60  c
61      data atol/1.0d-3/, rtol/0.0d0/
62  c
63      common /pcom/ dx, dy, coeffx, coeffy, coeffxy, uext,
64      &           nlocal, neq, mx, my, mxsub, mysub, npey, npex,
65      &           ixsub, jysub, thispe
66  c
67  c Initialize variables
68  c
69      npex = 2
70      npey = 2
71      mxsub = 5
72      mysub = 5
73      mx = npex*mxsub
74      my = npey*mysub
75      neq = mx*my
76      nlocal = mxsub*mysub
77      inopt = 1
78      t0 = 0.0d0
79      t1 = 0.01d0
80      mudq = mxsub
81      mldq = mxsub
82      mukeep = 1
83      mlkeep = 1
84      dqrely = 0.0d0
85      maxl = 0
86      gstype = 0
87      maxrs = 0
88      eplifac = 0.0d0
89      dqincfac = 0.0d0
90      itask = 1
91      iatol = 1
92  c
93  c Initialize MPI environment
94  c
95      call mpi_init(ier)
96      if (ier .ne. 0) then
97          write(*,2) ier
98      2      format(///' MPI_ERROR: MPI_INIT returned IER = ', i5)
99          stop
100     endif
101  c
102     call mpi_comm_size(MPI_COMM_WORLD, npes, ier)
103     if (ier .ne. 0) then
104         write(*,3) ier
105     3      format(///' MPI_ERROR: MPI_COMM_SIZE returned IER = ', i5)
106         call mpi_abort(MPI_COMM_WORLD, 1, ier)
107         stop
108     endif
109  c
110     call mpi_comm_rank(MPI_COMM_WORLD, thispe, ier)
111     if (ier .ne. 0) then
112         write(*,4) ier
113     4      format(///' MPI_ERROR: MPI_COMM_RANK returned IER = ', i5)
114         call mpi_abort(MPI_COMM_WORLD, 1, ier)
115         stop
116     endif

```

```

117  c
118      if (npes .ne. npex*npey) then
119          if (thispe .eq. 0) then
120              write(*,5) npes, npex*npey
121          5      format(///' MPI_ERROR: npes = ', i5, ' is not equal to ',
122              &           'NPEX*NPEY = ', i5)
123          call mpi_finalize(ier)
124          stop
125      endif
126  endif
127  c
128      call fnvinitp(MPI_COMM_WORLD, 2, nlocal, neq, ier)
129      if (ier .ne. 0) then
130          write(*,6) ier
131      6      format(///' SUNDIALS_ERROR: FNVINITP returned IER = ', i5)
132          call mpi_finalize(ier)
133          stop
134      endif
135  c
136      jysub = int(thispe/npex)
137      ixsub = thispe-jysub*npex
138  c
139  c Initialize problem data
140  c
141      call setinitprofile(uu, up, id, res, constr, ipar, rpar)
142  c
143  c Initialize IDA environment
144  c
145      call fidamalloc(t0, uu, up, iatol, rtol, atol,
146      &           iout, rout, ipar, rpar, ier)
147      if (ier .ne. 0) then
148          write(*,7) ier
149      7      format(///' SUNDIALS_ERROR: FIDAMALLOC returned IER = ', i5)
150          call mpi_abort(MPI_COMM_WORLD, 1, ier)
151          stop
152      endif
153  c
154  c Set optional inputs
155  c
156      call fidasetiin('SUPPRESS_ALG', 1, ier)
157      call fidasetvin('ID_VEC', id, ier)
158      call fidasetvin('CONSTR_VEC', constr, ier)
159
160  c
161  c Initialize and attach BBDSPGMR module
162  c
163      call fidabbdinit(nlocal, mudq, mldq, mukeep, mlkeep, dqrely, ier)
164      if (ier .ne. 0) then
165          write(*,8) ier
166      8      format(///' SUNDIALS_ERROR: FIDABBDINIT returned IER = ', i5)
167          call mpi_abort(MPI_COMM_WORLD, 1, ier)
168          stop
169      endif
170  c
171      call fidabbdspgmr(maxl, gstype, maxrs, eplifac, dqincfac, ier)
172      if (ier .ne. 0) then
173          write(*,9) ier
174      9      format(///' SUNDIALS_ERROR: FIDABBDSPGMR returned IER = ', i5)
175          call mpi_abort(MPI_COMM_WORLD, 1, ier)

```

```

176         stop
177     endif
178 c
179 c Print header
180 c
181     if (thispe .eq. 0) then
182         call prntintro(rtol, atol)
183         call prntcase(1, mudq, mukeep)
184     endif
185 c
186     tout = t1
187     do 10 jout = 1, nout
188 c
189         call fidasolve(tout, tret, uu, up, itask, ier)
190 c
191         call prntoutput(tret, uu, iout, rout)
192 c
193         if (ier .ne. 0) then
194             write(*,11) ier
195             11      format(///' SUNDIALS_ERROR: FIDASOLVE returned IER = ', i5)
196             call fidafree
197             stop
198         endif
199 c
200         tout = tout*2.0d0
201 c
202     10    continue
203 c
204 c Print statistics
205 c
206     if (thispe .eq. 0) then
207         call prntfinalstats(iout)
208     endif
209 c
210 c Reinitialize variables and data for second problem
211 c
212     mudq = 1
213     mldq = 1
214     jysub = thispe/npex
215     ixsub = thispe-jysub*npex
216 c
217     call setinitprofile(uu, up, id, res, constr, ipar, rpar)
218 c
219     call fidareinit(t0, uu, up, iatol, rtol, atol, ier)
220     if (ier .ne. 0) then
221         write(*,33) ier
222         33      format(///' SUNDIALS_ERROR: FIDAREINIT returned IER = ', i5)
223     endif
224 c
225     call fidabbdreinit(nlocal, mudq, mldq, dqrely, ier)
226     if (ier .ne. 0) then
227         write(*,34) ier
228         34      format(///' SUNDIALS_ERROR: FIDABBDREINIT returned IER = ', i5)
229         call fidafree
230         stop
231     endif
232 c
233 c Print header
234 c

```

```

235      if (thispe .eq. 0) then
236          call prntcase(2, mudq, mukeep)
237      endif
238      c
239      tout = t1
240      do 12 jout = 1, nout
241      c
242          call fidasolve(tout, tret, uu, up, itask, ier)
243      c
244          call prntoutput(tret, uu, iout, rout)
245      c
246          if (ier .ne. 0) then
247              write(*,13) ier
248          13 format(///' SUNDIALS_ERROR: FIDASOLVE returned IER = ', i5)
249          call fidafree
250          stop
251      endif
252      c
253          tout = tout*2.0d0
254      c
255      12 continue
256      c
257      c Print statistics
258      c
259          if (thispe .eq. 0) then
260              call prntfinalstats(iout)
261          endif
262      c
263      c Free memory
264      c
265          call fidabbdfree
266          call fidafree
267      c
268          call mpi_finalize(ier)
269      c
270          stop
271      end
272      c
273      c =====
274      c
275          subroutine setinitprofile(uu, up, id, res, constr, ipar, rpar)
276      c
277      c global variables
278      c
279          integer*4 nlocal, neq, npex, npey, mxsub, mysub, mx, my
280          integer*4 ixsub, jysub, ipar(*)
281          integer thispe
282          integer mxsubg, mysubg, nlocalg
283          parameter (mxsubg = 5, mysubg = 5)
284          parameter (nlocalg = mxsubg*mysubg)
285          double precision dx, dy, coeffx, coeffy, coeffxy, rpar(*)
286          double precision uext((mxsubg+2)*(mysubg+2))
287      c
288      c local variables
289      c
290          integer*4 i, iloc, j, jloc, offset, loc
291          integer*4 ixbegin, ixend, jybegin, jyend
292          integer reserr
293          double precision xfact, yfact

```

```

294     double precision uu(*), up(*), id(*), res(*), constr(*)
295   c
296     common /pcom/ dx, dy, coeffx, coeffy, coeffxy, uext,
297     &           nlocal, neq, mx, my, mxsub, mysub, npey, npex,
298     &           ixsub, jysub, thispe
299   c
300   c Initialize variables
301   c
302     dx = 1.0d0/dble(mx-1)
303     dy = 1.0d0/dble(my-1)
304     coeffx = 1.0d0/(dx*dx)
305     coeffy = 1.0d0/(dy*dy)
306     coeffxy = 2.0d0/(dx*dx)+2.0d0/(dy*dy)
307     ixbegin = mxsub*ixsub
308     ixend = mxsub*(ixsub+1)-1
309     jybegin = mysub*jysub
310     jyend = mysub*(jysub+1)-1
311   c
312     do 14 i = 1, nlocal
313       id(i) = 1.0d0
314   14 continue
315   c
316     jloc = 0
317     do 15 j = jybegin, jyend
318       yfact = dy*dble(j)
319       offset = jloc*mxsub
320       iloc = 0
321       do 16 i = ixbegin, ixend
322         xfact = dx*dble(i)
323         loc = offset+iloc
324         uu(loc+1) = 16.0d0*xfact*(1.0d0-xfact)*yfact*(1.0d0-yfact)
325         if (i .eq. 0 .or. i .eq. mx-1) then
326           id(loc+1) = 0.0d0
327         endif
328         if (j .eq. 0 .or. j .eq. my-1) then
329           id(loc+1) = 0.0d0
330         endif
331         iloc = iloc+1
332   16 continue
333     jloc = jloc+1
334   15 continue
335   c
336     do 17 i = 1, nlocal
337       up(i) = 0.0d0
338       constr(i) = 1.0d0
339   17 continue
340   c
341     call fidaresfun(0.0d0, uu, up, res, ipar, rpar, reserr)
342   c
343     do 18 i = 1, nlocal
344       up(i) = -1.0d0*res(i)
345   18 continue
346   c
347     return
348   end
349   c
350   c =====
351   c
352     subroutine fidaresfun(tres, u, up, res, ipar, rpar, reserr)

```

```

353  c
354  c global variables
355  c
356      integer*4 nlocal, neq, npex, npey, mxsub, mysub, mx, my
357      integer*4 ixsub, jysub, ipar(*)
358      integer thispe
359      integer mxsubg, mysubg, nlocalg
360      parameter (mxsubg = 5, mysubg = 5)
361      parameter (nlocalg = mxsubg*mysubg)
362      double precision dx, dy, coeffx, coeffy, coeffxy, rpar(*)
363      double precision uext((mxsubg+2)*(mysubg+2))
364  c
365  c local variables
366  c
367      integer reserr
368      double precision tres
369      double precision u(*), up(*), res(*)
370  c
371      common /pcom/ dx, dy, coeffx, coeffy, coeffxy, uext,
372      &           nlocal, neq, mx, my, mxsub, mysub, npey, npex,
373      &           ixsub, jysub, thispe
374  c
375      call fidacommfn(nlocal, tres, u, up, ipar, rpar, reserr)
376  c
377      call fidaglocfn(nlocal, tres, u, up, res, ipar, rpar, reserr)
378  c
379      return
380  end
381  c
382  c =====
383  c
384      subroutine fidacommfn(nloc, tres, u, up, ipar, rpar, reserr)
385  c
386      include "mpif.h"
387  c
388  c global variables
389  c
390      integer*4 nlocal, neq, npex, npey, mxsub, mysub, mx, my
391      integer*4 ixsub, jysub, ipar(*)
392      integer thispe
393      integer mxsubg, mysubg, nlocalg
394      parameter (mxsubg = 5, mysubg = 5)
395      parameter (nlocalg = mxsubg*mysubg)
396      double precision dx, dy, coeffx, coeffy, coeffxy, rpar(*)
397      double precision uext((mxsubg+2)*(mysubg+2))
398  c
399  c local variables
400  c
401      integer*4 nloc
402      integer reserr
403      double precision tres, u(*), up(*)
404  c
405      integer request(MPI_STATUS_SIZE)
406      double precision buffer(2*mysub)
407  c
408      common /pcom/ dx, dy, coeffx, coeffy, coeffxy, uext,
409      &           nlocal, neq, mx, my, mxsub, mysub, npey, npex,
410      &           ixsub, jysub, thispe
411  c

```

```

412      call brecvpost(request, mxsub, mysub, buffer)
413  c
414      call bsend(mxsub, mysub, u)
415  c
416      call brecvwait(request, mxsub, buffer)
417  c
418      return
419      end
420  c
421  c =====
422  c
423      subroutine fidaglocfn(nloc, tres, u, up, res, ipar, rpar, reserr)
424  c
425  c global variables
426  c
427      integer*4 nlocal, neq, npex, npey, mxsub, mysub, mx, my
428      integer*4 ixsub, jysub, ipar(*)
429      integer thispe
430      integer mxsubg, mysubg, nlocalg
431      parameter (mxsubg = 5, mysubg = 5)
432      parameter (nlocalg = mxsubg*mysubg)
433      double precision dx, dy, coeffx, coeffy, coeffxy, rpar(*)
434      double precision uext((mxsubg+2)*(mysubg+2))
435  c
436  c local variables
437  c
438      integer*4 nloc
439      integer reserr
440      double precision tres, u(*), up(*), res(*)
441  c
442      integer*4 i, lx, ly, offsetu, offsetue, locu, locue
443      integer*4 ixbegin, ixend, jybegin, jyend, mxsub2
444      double precision termx, termy, termctr
445  c
446      common /pcom/ dx, dy, coeffx, coeffy, coeffxy, uext,
447      &           nlocal, neq, mx, my, mxsub, mysub, npey, npex,
448      &           ixsub, jysub, thispe
449  c
450      mxsub2 = mxsub+2
451  c
452      do 19 i = 1, nlocal
453          res(i) = u(i)
454  19 continue
455  c
456      offsetu = 0
457      offsetue = mxsub2+1
458      do 20 ly = 0, mysub-1
459          do 21 lx = 0, mxsub-1
460              uext(offsetue+lx+1) = u(offsetu+lx+1)
461  21 continue
462      offsetu = offsetu+mxsub
463      offsetue = offsetue+mxsub2
464  20 continue
465  c
466      ixbegin = 0
467      ixend = mxsub-1
468      jybegin = 0
469      jyend = mysub-1
470      if (ixsub .eq. 0) then

```

```

471         ixbegin = ixbegin+1
472     endif
473     if (ixsub .eq. npex-1) then
474         ixend = ixend-1
475     endif
476     if (jysub .eq. 0) then
477         jybegin = jybegin+1
478     endif
479     if (jysub .eq. npey-1) then
480         jyend = jyend-1
481     endif
482 c
483     do 22 ly = jybegin, jyend
484         do 23 lx = ixbegin, ixend
485             locu = lx+ly*mxsub
486             locue = (lx+1)+(ly+1)*mxsub2
487             termx = coeffx*(uext(locue)+uext(locue+2))
488             termy = coeffy*(uext(locue-mxsub2+1)+uext(locue+mxsub2+1))
489             termctr = coeffxy*uext(locue+1)
490             res(locu+1) = up(locu+1)-(termx+termy-termctr)
491     23     continue
492   22     continue
493 c
494     return
495 end
496 c
497 c ======
498 c
499     subroutine bsend(dsizex, dsizey, uarray)
500 c
501     include "mpif.h"
502 c
503 c global variables
504 c
505     integer*4 nlocal, neq, npex, npey, mxsub, mysub, mx, my
506     integer*4 ixsub, jysub
507     integer thispe
508     integer mxsubg, mysubg, nlocalg
509     parameter (mxsubg = 5, mysubg = 5)
510     parameter (nlocalg = mxsubg*mysubg)
511     double precision dx, dy, coeffx, coeffy, coeffxy
512     double precision uext((mxsubg+2)*(mysubg+2))
513 c
514 c local variables
515 c
516     integer*4 dsizex, dsizey
517     double precision uarray(*)
518 c
519     integer ier
520     double precision bufleft(mysub), bufright(mysub)
521 c
522     common /pcom/ dx, dy, coeffx, coeffy, coeffxy, uext,
523     &           nlocal, neq, mx, my, mxsub, mysub, npey, npex,
524     &           ixsub, jysub, thispe
525 c
526     if (jysub .ne. 0) then
527         call mpi_send(uarray(1), dsizex, mpi_double_precision,
528         &           thispe-npex, 0, mpi_comm_world, ier)
529     endif

```

```

530  c
531      if (jysub .ne. npey-1) then
532          offsetu = (mysub-1)*dsizex
533          call mpi_send(uarray(offsetu+1), dsizex, mpi_double_precision,
534          &                      thispe+npex, 0, mpi_comm_world, ier)
535      endif
536  c
537      if (ixsub .ne. 0) then
538          do 24 ly = 0, mysub-1
539              offsetu = ly*dsizex
540              bufleft(ly+1) = uarray(offsetu+1)
541          24     continue
542          call mpi_send(bufleft(1), dsizey, mpi_double_precision,
543          &                      thispe-1, 0, mpi_comm_world, ier)
544      endif
545  c
546      if (ixsub .ne. npex-1) then
547          do 25 ly = 0, mysub-1
548              offsetu = ly*mxsub+(mxsub-1)
549              bufright.ly+1) = uarray(offsetu+1)
550          25     continue
551          call mpi_send(bufright(1), dsizey, mpi_double_precision,
552          &                      thispe+1, 0, mpi_comm_world, ier)
553      endif
554  c
555      return
556  end
557  c
558  c =====
559  c
560      subroutine brecvpost(request, dsizex, dsizey, buffer)
561  c
562      include "mpif.h"
563  c
564  c global variables
565  c
566      integer*4 nlocal, neq, npex, npey, mxsub, mysub, mx, my
567      integer*4 ixsub, jysub
568      integer thispe
569      integer mxsubg, mysubg, nlocalg
570      parameter (mxsubg = 5, mysubg = 5)
571      parameter (nlocalg = mxsubg*mysubg)
572      double precision dx, dy, coeffx, coeffy, coeffxy
573      double precision uext((mxsubg+2)*(mysubg+2))
574  c
575  c local variables
576  c
577      integer*4 dsizex, dsizey
578      integer request(*)
579      double precision buffer(*)
580  c
581      integer ier
582      integer*4 offsetue
583  c
584      common /pcom/ dx, dy, coeffx, coeffy, coeffxy, uext,
585      &                  nlocal, neq, mx, my, mxsub, mysub, npey, npex,
586      &                  ixsub, jysub, thispe
587  c
588      if (jysub .ne. 0) then

```

```

589         call mpi_irecv(uext(2), dsizex, mpi_double_precision,
590         &                      thispe-npex, 0, mpi_comm_world, request(1),
591         &                      ier)
592     endif
593 c
594     if (jysub .ne. npey-1) then
595         offsetue = (1+(mysub+1)*(mxsub+2))
596         call mpi_irecv(uext(offsetue+1), dsizex, mpi_double_precision,
597         &                      thispe+npex, 0, mpi_comm_world, request(2),
598         &                      ier)
599     endif
600 c
601     if (ixsub .ne. 0) then
602         call mpi_irecv(buffer(1), dsizey, mpi_double_precision,
603         &                      thispe-1, 0, mpi_comm_world, request(3),
604         &                      ier)
605     endif
606 c
607     if (ixsub .ne. npex-1) then
608         call mpi_irecv(buffer(1+mysub), dsizey, mpi_double_precision,
609         &                      thispe+1, 0, mpi_comm_world, request(4),
610         &                      ier)
611     endif
612 c
613     return
614 end
615 c
616 c =====
617 c
618     subroutine brecvwait(request, dsizex, buffer)
619 c
620     include "mpif.h"
621 c
622 c global variables
623 c
624     integer*4 nlocal, neq, npex, npey, mxsub, mysub, mx, my
625     integer*4 ixsub, jysub
626     integer thispe
627     integer mxsubg, mysubg, nlocalg
628     parameter (mxsubg = 5, mysubg = 5)
629     parameter (nlocalg = mxsubg*mysubg)
630     double precision dx, dy, coeffx, coeffy, coeffxy
631     double precision uext((mxsubg+2)*(mysubg+2))
632 c
633 c local variables
634 c
635     integer request(*)
636     integer*4 dsizex
637     double precision buffer(*)
638 c
639     integer*4 ly, dsizex2, offsetue
640     integer ier, status(MPI_STATUS_SIZE)
641 c
642     common /pcom/ dx, dy, coeffx, coeffy, coeffxy, uext,
643     &                  nlocal, neq, mx, my, mxsub, mysub, npey, npex,
644     &                  ixsub, jysub, thispe
645 c
646     dsizex2 = dsizex+2
647 c

```

```

648      if (jysub .ne. 0) then
649          call mpi_wait(request(1), status, ier)
650      endif
651      c
652      if (jysub .ne. npey-1) then
653          call mpi_wait(request(2), status, ier)
654      endif
655      c
656      if (ixsub .ne. 0) then
657          call mpi_wait(request(3), status, ier)
658          do 26 ly = 0, mysub-1
659              offsetue = (ly+1)*dsizex2
660              uext(offsetue+1) = buffer.ly+1)
661      26      continue
662      endif
663      c
664      if (ixsub .ne. npex-1) then
665          call mpi_wait(request(4), status, ier)
666          do 27 ly = 0, mysub-1
667              offsetue = (ly+2)*dsizex2-1
668              uext(offsetue+1) = buffer.ly+mysub+1)
669      27      continue
670      endif
671      c
672      return
673  end
674  c
675  c =====
676  c
677      subroutine prntoutput(tret, u, iout, rout)
678  c
679  c global variables
680  c
681      integer*4 nlocal, neq, npex, npey, mxsub, mysub, mx, my
682      integer*4 ixsub, jysub
683      integer thispe
684      integer mxsubg, mysubg, nlocalg
685      parameter (mxsubg = 5, mysubg = 5)
686      parameter (nlocalg = mxsubg*mysubg)
687      double precision dx, dy, coeffx, coeffy, coeffxy
688      double precision uext((mxsubg+2)*(mysubg+2))
689  c
690  c local variables
691  c
692      integer*4 iout(*), lenrwbbd, leniwbbd, ngebbd
693      double precision tret, umax, u(*), rout(*)
694  c
695      common /pcom/ dx, dy, coeffx, coeffy, coeffxy, uext,
696      &           nlocal, neq, mx, my, mxsub, mysub, npey, npex,
697      &           ixsub, jysub, thispe
698  c
699      call maxnorm(u, umax)
700  c
701      if (thispe .eq. 0) then
702          call fidabbdopt(lenrwbbd, leniwbbd, ngebbd)
703          write(*,28) tret, umax, iout(9), iout(3), iout(7),
704          &             iout(20), iout(4), iout(16), ngebbd, rout(2),
705          &             iout(18), iout(19)
706      28      format(' ', e10.4, ' ', e13.5, ' ', i1, ' ', i2,

```

```

707      &      , , i3, , i3, , , i2,'+',i2, , ,
708      &      i3, , , e9.2, , , i2, , , i3)
709      endif
710  c
711      return
712      end
713  c
714  c =====
715  c
716      subroutine maxnorm(u, unorm)
717  c
718      include "mpif.h"
719  c
720  c global variables
721  c
722      integer*4 nlocal, neq, npex, npey, mxsub, mysub, mx, my
723      integer*4 ixsub, jysub
724      integer thispe
725      integer mxsubg, mysubg, nlocalg
726      parameter (mxsubg = 5, mysubg = 5)
727      parameter (nlocalg = mxsubg*mysubg)
728      double precision dx, dy, coeffx, coeffy, coeffxy
729      double precision uext((mxsubg+2)*(mysubg+2))
730  c
731  c local variables
732  c
733      integer*4 i
734      integer ier
735      double precision temp, unorm, u(*)
736  c
737      common /pcom/ dx, dy, coeffx, coeffy, coeffxy, uext,
738      &          nlocal, neq, mx, my, mxsub, mysub, npey, npex,
739      &          ixsub, jysub, thispe
740  c
741      temp = 0.0d0
742  c
743      do 29 i = 1, nlocal
744          temp = max(abs(u(i)), temp)
745  29 continue
746  c
747      call mpi_allreduce(temp, unorm, 1, mpi_double_precision,
748      &                      mpi_max, mpi_comm_world, ier)
749  c
750  c      unorm = temp
751  c
752      return
753      end
754  c
755  c =====
756  c
757      subroutine prntintro(rtol, atol)
758  c
759  c global variables
760  c
761      integer*4 nlocal, neq, npex, npey, mxsub, mysub, mx, my
762      integer*4 ixsub, jysub
763      integer thispe
764      integer mxsubg, mysubg, nlocalg
765      parameter (mxsubg = 5, mysubg = 5)

```

```

766     parameter (nlocalg = mxsubg*mysubg)
767     double precision dx, dy, coeffx, coeffy, coeffxy
768     double precision uext((mxsubg+2)*(mysubg+2))
769   c
770   c local variables
771   c
772     double precision rtol, atol
773   c
774     common /pcom/ dx, dy, coeffx, coeffy, coeffxy, uext,
775     &           nlocal, neq, mx, my, mxsub, mysub, npey, npex,
776     &           ixsu, jysu, thispe
777   c
778     write(*,30) mx, my, neq, mxsub, mysub, npex, npey, rtol, atol
779   30  format(/'fidakryx_bbd_p: Heat equation, parallel example problem',
780     &       ' for FIDA', /, 16x,'Discretized heat equation',
781     &       ' on 2D unit square.', /, 16x,'Zero boundary',
782     &       ' conditions, polynomial conditions.', /,
783     &       16x,'Mesh dimensions: ', i2, ' x ', i2,
784     &       '          Total system size: ', i3, //,
785     &       'Subgrid dimensions: ', i2, ' x ', i2,
786     &       '          Processor array: ', i2, ' x ', i2, '/',
787     &       'Tolerance parameters: rtol = ', e8.2, '    atol = ',
788     &       e8.2, /, 'Constraints set to force all solution',
789     &       ' components >= 0.', /, 'SUPPRESSALG = TRUE to remove',
790     &       ' boundary components from the error test.', /,
791     &       'Linear solver: SPGMR.    Preconditioner: BBDPRE - ',
792     &       'Banded-block-diagonal.')
793   c
794     return
795   end
796   c
797   c =====
798   c
799     subroutine prntcase(num, mudq, mukeep)
800   c
801   c local variables
802   c
803     integer*4 mudq, mukeep
804     integer num
805   c
806     write(*,31) num, mudq, mukeep
807   31  format(//, 'Case ', i2, /, ' Difference quotient half-',
808     &       'bandwidths =', i2, /, ' Retained matrix half-bandwidths =',
809     &       i2, //, 'Output Summary',/, ' umax = max-norm of solution',
810     &       /, ' nre = nre + nreLS (total number of RES evals.)',
811     &       //, ' time         umax      k nst  nni  nli  nre',
812     &       ' nge      h      npe  nps', /,
813     &       '-----', '-----',
814     &       '-----')
815   c
816     return
817   end
818   c
819   c =====
820   c
821     subroutine prntfinalstats(iout)
822   c
823   c local variables
824   c

```

```
825      integer*4 iout(*)
826      c
827      write(*,32) iout(5), iout(6), iout(21)
828      32    format(/, 'Error test failures      =', i3, /,
829      &      'Nonlinear convergence failures =', i3, /,
830      &      'Linear convergence failures   =', i3)
831      c
832      return
833      end
```

